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Preliminary Scoring of Selected Organic Air Pollutants. Appendix I. Chemistry Production, and Toxicity of Chemicals A - C

MITRE Corp, McLean, Va METREK Div

Prepared for

Environmental Protection Agency, Research Triangle Park, N C Office of Air Quality Planning and Standards

Oct 76

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October 1976

PRELIMINARY SCORING OF SELECTED ORGANIC AIR POLLUTANTS

APPENDIX I - CHEMISTRY, PRODUCTION, AND TOXICITY OF CHEMICALS A THROUGH C

U.S. ENVIRONMENTAL PROTECTION AGENCY
Office of Air and Waste Management
Office of Air Quality Planning and Standards
Research Triangle Park, North Carolina 27711

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This is the first of a series of four appendices to the report "Scoring of Organic Air Pollutants." The entire appendix contains a compilation of available data on chemical structure and properties, environmental persistence, production, and toxicity for 637 synthetic organic chemicals.

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by

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Contract No. 68-02-1495

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EPA Project Officer: David R. Patrick

Prepared for

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Office of Air and Waste Management
Office of Air Quality Planning and Standards
Research Triangle Park, North Carolina 27711

October 1976

1-A

PREFACE

A program is being developed by the Emission Standards and Engineering Division of the U.S. Environmental Protection Agency to determine the extent and environmental effects of atmospheric industrial emissions of synthetic organic chemicals. As part of the initial effort, EPA requested that the MITRE Corporation, METREK Division, devise a system for identifying those chemicals that may be released to the atmosphere from chemical manufacturing plants and whose health effects have been documented. To address this need, three general categories of information for each compound to be evaluated were deemed directly relevant:

(1) the quantity of the compound produced;

(2) the potential for atmospheric release from chemical manufacturing plants, and

(3) the toxicological effects of the compounds.

The results of this study are presented in the accompanying report "Preliminary Scoring of Organic Air Pollutants."

The following dossiers were prepared for each of the 637 compounds under consideration in an attempt to collate the pertinent data for subsequent evaluation.

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APPENDIX I

CHEMISTRY, PRODUCTION AND TOXICITY OF SELECTED SYNTHETIC ORGANIC CHEMICALS

Acenapthene

CHEMICAL NAME

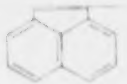
CAS Number: 208-96-8

Chemical Name: Acenaphthlylene

Synonyms: 1,2-Dihydro-acenaphthylene
1,8-Ethylene naphthalene
Naphthyleneethylene

Molecular Formula: $C_{12}H_8$

Structure:



Chemical Properties

Molecular Weight: 154.21

Physical State: Solid

Vapor Pressure: 10 mm at 131.2°C

Vapor Density: 5.32

Boiling Point: 277.5°C

Melting Point: 96.2°C

Density: 1.0242 at 99°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire-slight

Acenapthene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Non-lethal Acute Effects:
Irritant to skin and mucous membranes

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Neoplastic effects

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Acetal

CHEMICAL NAME

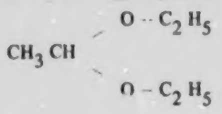
CAS Number: 105-57-7

Chemical Name: Diethyl acetal acetaldehyde

Synonyms: 1,1-Diethoxyethane
Ethylidene diethyl ether
Diethylacetal

Molecular Formula: $C_6H_{14}O_2$

Structure:



$$CH_3CH\begin{matrix} O-C_2H_5 \\ O-C_2H_5 \end{matrix}$$

Chemical Properties

Molecular Weight: 118.18

Vapor Pressure: 28.8 at 25°C

Boiling Point: 103.2°C at 760 mm

Density: 0.8314 at 20°C/4°C

Octanol/Water Partition Coefficient: 1.17

Physical State: Liquid

Vapor Density: 4.08 mp at 100°C

Melting Point:

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–dangerous
Explosion–moderate

PRODUCTION DATA

Annual U.S. Production: 56.8×10^6 lbs. (1975)

Consumption: 60.4×10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 63.3

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	4570 mg/kg	rat	oral
LC_{Lo}	4000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Narcotic

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Acetaldehyde

CHEMICAL NAME

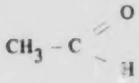
CAS Number: 75-07-0

Chemical Name: Acetaldehyde

Synonyms: Acetic aldehyde
Ethyl aldehyde

Molecular Formula: C_2H_4O

Structure:



$CH_3-C\overset{\displaystyle O}{\underset{\displaystyle H}{\diagup\!\!\diagdown}}$

Chemical Properties

Molecular Weight: 44.05

Vapor Pressure: 923 Torrs at 25°C

Boiling Point: 20.8°C at 760 mm

Density: 0.7834 at 18°C/4°C

Octanol/Water Partition Coefficient: 0.43

Physical State: Liquid

Vapor Density: 1 [illegible]

Melting Point: -121°C

Solubility: Infinite (hot H_2O)

Environmental Persistence

BOD: 126 at 20°C for 5 days

Atmospheric Reactivity:

Safety Hazard: Fire–dangerous–oxidizes
Explosion–severe

Acetaldehyde

PRODUCTION DATA

Annual U.S. Production: 1500 x 10^6 lbs. (1976)

Consumption: 1300 x 10^6 lbs. (1976)

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 36.2

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1930 mg/kg	rat	oral
	640 mg/kg	rat	subcutaneous
	1232 mg/kg	mouse	oral
	560 mg/kg	mouse	subcutaneous
LD_{Lo}	500 mg/kg	rat	intraperitoneal
LC_{Lo}	4000 ppm (4 hours)	rat	inhalation
Non-lethal Acute Effects:			
TC_{Lo}	134 ppm	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: TWA–200 ppm

Carcinogenicity:			
TD_{Lo}	60 mg/kg (79 weeks)	rat	subcutaneous

Mutagenicity:

Teratogenicity:

TLV: 200 ppm

Other Chronic Effects:

Eye irritation 50 ppm

Acetaldol

CHEMICAL NAME

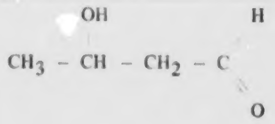
CAS Number: 107-89-1

Chemical Name: 3-Hydroxybutyraldehyde

Synonyms:
Acetaldol
Aldol
3-Butanolal
Oxybutyric aldehyde

Molecular Formula: $C_4H_8O_2$

Structure:



$$\mathrm{CH_3 - \overset{OH}{\overset{|}{CH}} - CH_2 - \overset{H}{\underset{O}{C}}}$$

Chemical Properties

Molecular Weight: 88.12

Physical State: Liquid

Vapor Pressure: 10 mm at 25°C

Vapor Density: 3.04

Boiling Point: 83°C at 20 mm
Decomposes at 85°C

Melting Point:

Density: 1.103 at 20°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–moderate

Acetaldol

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	2,180 mg/kg	rat	oral
	140 mg/kg	rat	skin

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Acetamide

CHEMICAL NAME

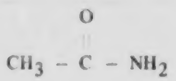
CAS Number: 60-35-5

Chemical Name: Acetamide

Synonyms: Acetic acid amide
Ethanamide

Molecular Formula: C_2H_5NO

Structure:



$$CH_3 - \overset{\overset{\displaystyle O}{\|}}{C} - NH_2$$

Chemical Properties

Molecular Weight: 59.07

Vapor Pressure: 1 mm at 65°C

Boiling Point: 221.2°C at 760 mm

Density: 1.1590 at 20°C/4°C

Octanol/Water Partition Coefficient: -1.46

Physical State: Solid

Vapor Density:

Melting Point: 82.3°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous–cyanide

Acetamide

CHEMICAL NAME

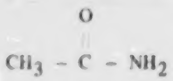
CAS Number: 60-35-5

Chemical Name: Acetamide

Synonyms: Acetic acid amide
Ethanamide

Molecular Formula: C_2H_5NO

Structure:



$$CH_3 - \overset{\overset{\displaystyle O}{\|}}{C} - NH_2$$

Chemical Properties

Molecular Weight:	59.07	**Physical State:**	Solid
Vapor Pressure:	1 mm at 65°C	**Vapor Density:**	
Boiling Point:	221.2°C at 760 mm	**Melting Point:**	82.3°C
Density:	1.1590 at 20°C/4°C	**Solubility:**	Soluble (H_2O)
Octanol/Water Partition Coefficient:	-1.46		

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous–cyanide

Acetamide

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	10 gm/kg	rat	subcutaneous
	8300 mg/kg	mouse	subcutaneous

Non-lethal Acute Effects:
Mild irritant

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

TD_{Lo}	456 gm/kg (52 weeks)	rat	oral

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Acetamidofluorene

CHEMICAL NAME

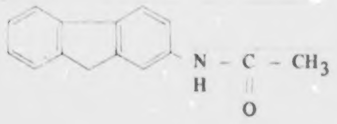
CAS Number: 53-96-3

Chemical Name: N-fluoren-2-yl-acetamide

Synonyms: 2-Acetamidofluorene
N-(2-fluorenyl)acetamide
2-Acetylaminofluorene

Molecular Formula: $C_{15}H_{13}NO$

Structure:



Chemical Properties

Molecular Weight: 223.28

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 194°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Acetamidofluorene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD$_{50}$	1020 mg/kg	mouse	oral

Chronic Toxicity

U.S. Occupational Standard: (air) Carcinogen

Carcinogenicity:

TD$_{Lo}$	15 gm/kg (4 weeks)	hamster	intravenous
	475 mg/kg (11 weeks)	rat	oral
	260 mg/kg (1 week)	rat	skin
	192 mg/kg (8 weeks)	rat	intraperitoneal
	560 mg/kg (14 days)	mouse	oral
	4400 mg/kg (65 weeks)	rabbit	oral
	7980 mg/kg (38 weeks)	hamster	oral

Mutagenicity:

Teratogenicity: **TLV:**

TD$_{Lo}$	100 mg/kg	mouse	parenteral

Other Chronic Effects:

Acetanilide

CHEMICAL NAME

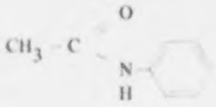
CAS Number: 103-84-4

Chemical Name: Acetanilide

Synonyms: N-phenylacetamide
Antifibrin

Molecular Formula: C_8H_9NO

Structure:



Chemical Properties

Molecular Weight: 135.17

Vapor Pressure: 1 mm at 114°C

Boiling Point: 303.8°C at 760 mm

Density: 1.2190 at 15°C/4°C

Octanol/Water Partition Coefficient: 1.59

Physical State: Solid

Vapor Density: 4.65

Melting Point: 114.3°C

Solubility: Slightly soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–slight

Acetanilide

PRODUCTION DATA

Annual U.S. Production: 5.5 x 10^6 lbs. (1967)

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	800 mg/kg	rat	oral
	1210 mg/kg	mouse	oral
LD_{Lo}	1000 mg/kg	mouse	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Acetic Acid

CHEMICAL NAME

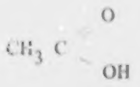
CAS Number: 64-19-7

Chemical Name: Acetic acid

Synonyms:
Methane carboxylic acid
Ethylic acid
Glacial acetic acid
Ethanoic acid
Vinegar acid

Molecular Formula: $C_2H_4O_2$

Structure:



$$CH_3C\begin{matrix}\nearrow O\\ \searrow OH\end{matrix}$$

Chemical Properties

Molecular Weight: 60.05

Physical State: Liquid

Vapor Pressure: 11.4 mm at 20°C

Vapor Density: 2.07

Boiling Point: 117.9°C at 760 mm

Melting Point: 16.6°C

Density: 1.0492 at 20°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient: –0.31

Environmental Persistence

BOD: 102.7 at 20°C for 20 days

Atmospheric Reactivity:

Safety Hazard:
Fire–moderate
Explosion–moderate

Acetic Acid

PRODUCTION DATA

Annual U.S. Production: 2097.0 x 10^6 lbs. (1975)

Consumption: 2097.6 x 10^6 lbs.

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 55.9

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3310 mg/kg	rat	oral
	4960 mg/kg	mouse	oral
	525 mg/kg	mouse	intravenous
LD_{Lo}	1200 mg/kg	rabbit	oral
	1200 mg/kg	rabbit	subcutaneous
	600 mg/kg	rabbit	rectal
LC_{50}	5620 ppm (1 hour)	mouse	inhalation
Non-lethal Acute Effects:			
Irritant – LD_{Lo}	816 ppm (3 months)	human	inhalation
	50 ppm	human	inhalation
Gastrointestinal tract – LD_{Lo}	1470 mg/kg	human	oral

Chronic Toxicity

U.S. Occupational Standard: TWA – 10 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 10 ppm

Other Chronic Effects:

- Dermatitis
- Ulcers
- Slight irritation of respiratory tract 100-260 ppm (1 hour)
- Conjuctivitis
- Bronchitis, pharyngitis
- Erosion of exposed teeth

Acetic anhydride

CHEMICAL NAME

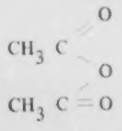
CAS Number: 108-24-7

Chemical Name: Acetic anhydride

Synonyms: Acetyl oxide
Acetic oxide
Ethanoic anhydride

Molecular Formula: $C_4H_6O_3$

Structure:



Chemical Properties

Molecular Weight: 102.09

Vapor Pressure: 5.09 mm at 25°C

Boiling Point: 139.55°C

Density: 1.082 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 3.50

Melting Point: -73.1°C

Solubility: Very soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–moderate
Explosion–moderate

Acetic anhydride

PRODUCTION DATA

Annual U.S. Production: 1633.1 x 10^6 lbs. (1974)

Consumption: 1637 x 10^6 lbs.

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 39.4

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1780 mg/kg	rat	oral
LC_{Lo}	1000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Irritant to eyes and upper respiratory tract

Ingestion–burning pain in stomach followed by nausea and vomiting

Chronic Toxicity

U.S. Occupational Standard: TWA: 5 ppm (air)

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 5 ppm

Other Chronic Effects:

Acetone

CHEMICAL NAME

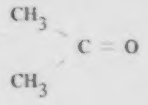
CAS Number: 67-64-1

Chemical Name: Acetone

Synonyms:
2-Propanone
Dimethyl ketone
β-Ketone propane
Methylketone
Pyroacetic ether

Molecular Formula: C_3H_6O

Structure:



Chemical Properties

Molecular Weight: 58.08

Vapor Pressure: 400 mm at 39.5°C

Boiling Point: 56.2°C at 760 mm

Density: 0.7972 at 15°C/4°C

Octanol/Water Partition Coefficient: 0.55

Physical State: Liquid

Vapor Density: 2.0

Melting Point: -95.35°C

Solubility: Infinite (H_2O)

Environmental Persistence

BOD: 1.84 for 20 days at 20°C
72% of theoretical for 10 days at 20°C

Atmospheric Reactivity: Oxygen uptake: 50 mg/l during 12 hours

Safety Hazard: Fire–dangerous
Explosion–moderate

Acetone

PRODUCTION DATA

Annual U.S. Production: 1980.3×10^6 lbs. (1974)

Consumption: 1946.0×10^6 lbs.

Fraction of Dispersion: 0.31

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 533.9

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1295 mg/kg	mouse	intraperitoneal
	5300 mg/kg	rabbit	oral
LD_{Lo}	8000 mg/kg	dog	oral
Non-lethal Acute Effects:			
Eye effects–TC_{Lo}	500 ppm	human	air exposure
Central nervous system TC_{Lo}	12,000 ppm (4 hours)		
Paralysis			

Chronic Toxicity

U.S. Occupational Standard: TWA: 1000 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 1000 ppm

Other Chronic Effects:

Skin irritation	**Odor perception:**	1.6 ppm
Chronic respiratory tract irritation, dizziness	1000 ppm (3 hours/day)	
Minor irritation of eyes and nose	3000 ppm	

Acetone cyanohydrin

CHEMICAL NAME

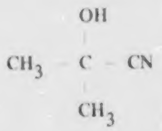
CAS Number: 75-86-5

Chemical Name: 2-Methyl lactonitrile

Synonyms: Hydroxyisobutyronitrile

Molecular Formula: C_4H_7NO

Structure:



$$CH_3 - \overset{\displaystyle OH}{\underset{\displaystyle CH_3}{C}} - CN$$

Chemical Properties

Molecular Weight: 85.11

Vapor Pressure:

Boiling Point: 82°C at 23 mm

Density: 0.932 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 2.93

Melting Point: -20°C

Solubility: Very soluble, decomposes in H_2O

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire - slight

Acetone cyanohydrin

PRODUCTION DATA

Annual U.S. Production: 537.9×10^6 lbs (1969)

Consumption: 100×10^6 lbs (1975)

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 6.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	17 mg/kg	rat	oral
	3 mg/kg	mouse	oral
	14 mg/kg	rabbit	oral
	17 mg/kg	rabbit	skin
	9 mg/kg	guinea pig	oral
LC_{50}	575 ppm (2 hours)	mouse	inhalation
LC_{Lo}	63 ppm (4 hours)	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: Unconfirmed

Other Chronic Effects:

Acetonitrile

CHEMICAL NAME

CAS Number: 75-05-8

Chemical Name: Acetonitrile

Synonyms:	Methyl cyanide Cyanomethane Ethanenitrile	Ethyl nitrile Methane carbonitrile

Molecular Formula: C_2H_3N

Structure: $CH_3 - C \equiv N$

Chemical Properties

Molecular Weight: 41.05	**Physical State:** Liquid
Vapor Pressure: 92.8 mm at 25°C	**Vapor Density:** 1.42
Boiling Point: 81.6°C	**Melting Point:** −45.72°C
Density: 0.786 at 20°C/20°C	**Solubility:** Infinite (H_2O)
Octanol/Water Partition Coefficient: −0.34	

Environmental Persistence

BOD: Total theoretical oxygen demand 3.32

Atmospheric Reactivity: Reacts to oxidizing materials

Safety Hazard: Fire–dangerous
Disaster hazard–dangerous, toxic fumes (HCN)

Acetonitrile

PRODUCTION DATA

Annual U.S. Production: 135 x 10^6 lbs.

Consumption: 135 x 10^6 lbs.

Fraction of Dispersion: 0.50

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 69.5

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3800 mg/kg	rat	oral
	1920 mg/kg	mouse	intraperitoneal
LD_{Lo}	700 mg/kg	mouse	subcutaneous
LC_{Lo}	8000 ppm (4 hours)	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard: TWA: 40 ppm

Carcinogenicity: Equivocal results from 2-year rat study.

Mutagenicity:

Teratogenicity: Fetal malformations in rats, 0.2 to 1.0 ml/kg intraperitoneal

TLV: 40 ppm

Other Chronic Effects:
Growth retardation
Metabolic disturbances
Liver enlargement

Acetophenone

CHEMICAL NAME

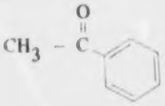
CAS Number: 98-86-2

Chemical Name: Acetophenone

Synonyms:
1-Phenyl-ethanone
Methyl phenyl ketone
Phenyl methyl ketone
Acetylbenzene
Hypnone

Molecular Formula: C_8H_8O

Structure:



Chemical Properties

Molecular Weight: 120.16

Vapor Pressure: 1 mm at 37.1°C

Boiling Point: 202.0°C

Density: 1.0281 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid or solid

Vapor Density: 4.14

Melting Point: 20.5°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–slight

Acetophenone

PRODUCTION DATA

Annual U.S. Production:	2.68×10^6 lbs.	**Consumption:**	
Fraction of Dispersion:	0.01	**Fraction of Production Lost:**	0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	900 mg/kg	rat	oral
LD_{Lo}	200 mg/kg	mouse	intraperitoneal

Non-lethal Acute Effects:

Dermatitis
Narcosis
CNS depressant

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Acetylene

CHEMICAL NAME

CAS Number: 74-86-2

Chemical Name: Acetylene

Synonyms: Ethyne
Ethine

Molecular Formula: C_2H_2

Structure: $HC \equiv CH$

Chemical Properties

Molecular Weight: 26.04

Vapor Pressure: 5600 mm at 16.8°C

Boiling Point: -84.0°C at 760 mm (sublimes)

Density: 0.6181 at -32°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Gas

Vapor Density: 0.91

Melting Point: -80.8°C

Solubility: Slight (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–dangerous
Explosion–moderate

Acetylene

PRODUCTION DATA

Annual U.S. Production: 538×10^6 lbs. (1974)

Consumption: 617×10^6 lbs.

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 9.1

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LC_{Lo}	90,000 ppm	rat	inhalation

Non-lethal Acute Effects:

- Nausea
- Cyanosis
- CNS depression

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Intoxication:	100,000 ppm	man (slight)
	200,000 ppm	man (marked)
Incoordination:	300,000 ppm	man
Unconsciousness:	350,000 ppm (5 minutes)	man

Acetylene tetrabromide

CHEMICAL NAME

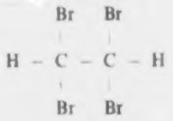
CAS Number: 79-27-6

Chemical Name: 1,1,2,2-Tetrabromoethane

Synonyms: Acetylenetetrabromide
Muthmann's liquid

Molecular Formula: $C_2H_2Br_4$

Structure:



$$\begin{array}{ccccccc} & & \mathrm{Br} & & \mathrm{Br} & & \\ & & | & & | & & \\ \mathrm{H} & - & \mathrm{C} & - & \mathrm{C} & - & \mathrm{H} \\ & & | & & | & & \\ & & \mathrm{Br} & & \mathrm{Br} & & \end{array}$$

Chemical Properties

Molecular Weight: 345.67

Vapor Pressure: 1 mm at 65°C

Boiling Point: 243.5°C at 760 mm

Density: 2.9656 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point: 0°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous–toxic fumes of carbonyl bromide when heated

Acetylene tetrabromide

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	400 mg/kg	rabbit	oral
	400 mg/kg	guinea pig	oral

Non-lethal Acute Effects:

Irritant
Narcotic

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 1 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Acetylene tetrachloride

CHEMICAL NAME

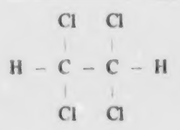
CAS Number: 79-34-5

Chemical Name: 1,1,2,2,-Tetrachloroethane

Synonyms: Acetylene tetrachloride

Molecular Formula: $C_2H_2Cl_4$

Structure:



$$\begin{array}{ccccccc} & & Cl & & Cl & & \\ & & | & & | & & \\ H & - & C & - & C & - & H \\ & & | & & | & & \\ & & Cl & & Cl & & \end{array}$$

Chemical Properties

Molecular Weight: 167.85	Physical State: Liquid
Vapor Pressure: 6.75 mm at 25°C	Vapor Density:
Boiling Point: 146.2°C at 760 mm	Melting Point: -43.8°C
Density: 1.5953 at 20°C/4°C	Solubility: Slightly (H_2O)
Octanol/Water Partition Coefficient:	

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Explosion–moderate if contact with Na or K

Acetylene tetrachloride

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{Lo}	30 mg/kg	mouse	intraperitoneal
	700 mg/kg	dog	oral
	50 mg/kg	dog	intravenous
	500 mg/kg	rabbit	subcutaneous
LC_{Lo}	1000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Central nervous system			
TD_{Lo}	30 mg/kg	human	oral

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 5 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Acrolein

CHEMICAL NAME

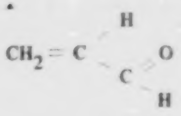
CAS Number: 107-02-8

Chemical Name: Acrolein

Synonyms:
2-Propenal
Acrylic aldehyde
Allyl aldehyde
Acraldehyde

Molecular Formula: C_3H_4O

Structure:



Chemical Properties

Molecular Weight: 56.06

Vapor Pressure: 288.2 mm at 25°C

Boiling Point: 52.5°C

Density: 0.8410 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 1.94

Melting Point: -86.95°C

Solubility: Very soluble, (400,000 mg/l of H_2O)

Environmental Persistence

BOD: 33% of theoretical after 10 days

Atmospheric Reactivity: Reactive with oxidizing materials

Safety Hazard: Fire–dangerous

Acrolein

PRODUCTION DATA

Annual U.S. Production: 61.73 x 10^6 lbs.

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	46 mg/kg	rat	oral
	50 mg/kg	rat	subcutaneous
	30 mg/kg	mouse	subcutaneous
	7 mg/kg	rabbit	oral
	562 mg/kg	rabbit	skin
LD_{Lo}	2 mg/kg	mouse	intraperitoneal
	150 mg/kg	rabbit	subcutaneous
	150 mg/kg	guinea pig	subcutaneous
LC_{Lo}	153 ppm (10 minutes)	human	inhalation
	8 ppm (4 hours)	rat	inhalation
	24 mg/m^3 (6 hours)	mouse	inhalation
	1570 mg/m^3 (8 hours)	cat	inhalation
	24 mg/m^3 (6 hours)	rabbit	inhalation
	24 mg/m^3 (6 hours)	guinea pig	inhalation

Chronic Toxicity

U.S. Occupational Standard: TWA: 0.1 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 0.1 ppm

Other Chronic Effects:
Lachrymation
Irritant to respiratory tract
CNS damage

Acrylamide

CHEMICAL NAME

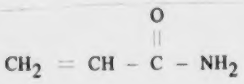
CAS Number: 79-06-1

Chemical Name: Acrylamide

Synonyms: Propenoic acid, amide
Propenamide
Acrylic amide

Molecular Formula: C_3H_5NO

Structure:



$CH_2 = CH - \overset{\displaystyle O}{\overset{\|}{C}} - NH_2$

Chemical Properties

Molecular Weight:	71.08	**Physical State:**	Solid
Vapor Pressure:	1.6 mm at 84.5°C	**Vapor Density:**	
Boiling Point:	125°C at 25 mm	**Melting Point:**	84 to 85°C
Density:	1.122 at 30°C	**Solubility:**	Very soluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–moderate–emits acrid fumes

Acrylamide

PRODUCTION DATA

Annual U.S. Production: 35 x 10^6 lbs.

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	170 mg/kg	rat	oral
	170 mg/kg	mouse	oral
LD_{Lo}	126 mg/kg	rabbit	oral
	1000 mg/kg	rabbit	skin
	252 mg/kg	guinea pig	oral

Non-lethal Acute Effects:

CNS paralysis

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 0.3 mg/m^3

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 0.3 mg/m^3 (skin)

Other Chronic Effects:

Acrylic acid

CHEMICAL NAME

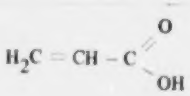
CAS Number: 79-10-7

Chemical Name: Acrylic acid

Synonyms: Acroleic acid
Propene acid
2-Propenoic acid

Molecular Formula: $C_3H_4O_2$

Structure:



$H_2C=CH-C(=O)OH$

Chemical Properties

Molecular Weight: 72.06

Vapor Pressure: 4.61 mm at 25°C

Boiling Point: 141°C

Density: 1.0511 at 20°C/4°C

Octanol/Water Partition Coefficient: 0.43

Physical State: Liquid

Vapor Density: 2.45

Melting Point: 13°C

Solubility: Infinite (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing material

Safety Hazard: Fire–slight
Explosion–moderate, spontaneous polymerization
Disaster hazard–dangerous, toxic fumes

Acrylic acid

PRODUCTION DATA

Annual U.S. Production:	233 x 10^6 lbs. (1974)	**Consumption:**	
Fraction of Dispersion:	0.01	**Fraction of Production Lost:**	0.015

Release Rate (million lbs/yr): 2.7

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	340 mg/kg	rat	oral
	60 mg/kg	mouse	oral
	280 mg/kg	rabbit	skin
LD_{Lo}	128 mg/kg	mouse	intraperitoneal
LC_{Lo}	6000 ppm (5 hours)	rat	inhalation

Non-lethal Acute Effects:

Irritant to eyes and skin

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: unconfirmed

Other Chronic Effects:

Acrylonitrile

CHEMICAL NAME

CAS Number: 107-13-1

Chemical Name: Acrylonitrile

Synonyms: 2-Propenenitrile
Vinyl cyanide

Molecular Formula: C_3H_3N

Structure: $CH_2 = CH - C \equiv N$

Chemical Properties

Molecular Weight: 53.00

Vapor Pressure: 113.8 mm at 25°C

Boiling Point: 77.5°C

Density: 0.8060 at 20°C/4°C

Octanol/Water Partition Coefficient: –0.92

Physical State: Liquid

Vapor Density: 1.83

Melting Point: –83 to –84°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–dangerous
Explosion–moderate

Acrylonitrile

PRODUCTION DATA

Annual U.S. Production: 1411.8 x 10^6 lbs. (1974)

Consumption: 511.7 x 10^6 lbs. (1974)

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 27.4 (1972)

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	93 mg/kg	rat	oral
	96 mg/kg	rat	subcutaneous
	93 mg/kg	rabbit	oral
	280 mg/kg	rabbit	skin
	250 mg/kg	guinea pig	skin
LD_{Lo}	15 mg/kg	mouse	intraperitoneal
LC_{100}	784 ppm (1 hour)	mouse	inhalation
LC_{50}	576 ppm (4 hours)	guinea pig	inhalation
LC_{Lo}	500 ppm (4 hours)	rat	inhalation
	120 mg/kg (4 hours)	dog	inhalation
	600 ppm (4 hours)	cat	inhalation
	258 ppm (4 hours)	rabbit	inhalation

Chronic Toxicity

U.S. Occupational Standard: TWA: 20 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 20 ppm (skin)

Other Chronic Effects:
Inhibits respiratory enzyme
Irritation of eyes and nose
Anemia and leucocytosis
Affects liver and kidney

Odor perception: 21.4 ppm

Adipic acid

CHEMICAL NAME

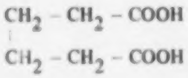
CAS Number: 124-04-9

Chemical Name: Adipic acid

Synonyms: Hexanedioic acid
1,4-Butane dicarboxylic acid
Adipinic acid

Molecular Formula: $C_6H_{10}O_4$

Structure:



$$\begin{array}{l} CH_2 - CH_2 - COOH \\ | \\ CH_2 - CH_2 - COOH \end{array}$$

Chemical Properties

Molecular Weight: 146.14

Physical State: Solid

Vapor Pressure: 1 mm at 159.5°C

Vapor Density: 5.04

Boiling Point: 337.5°C

Melting Point: 153°C

Density: 1.360 at 25°C/4°C

Solubility: Slightly, (15 gm/l of H_2O)

Octanol/Water Partition Coefficient: -0.14

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–slight

Adipic acid

PRODUCTION DATA

Annual U.S. Production: 1478.4 x 10^6 lbs. (1974)

Consumption: 1475 x 10^6 lbs.

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 37.3

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1900 mg/kg	mouse	oral
LD_{Lo}	3600 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Alachlor

CHEMICAL NAME

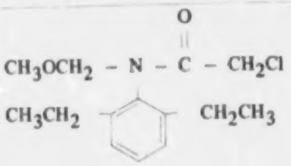
CAS Number: 15972-60-8

Chemical Name: 2-Chloro-N-(2,6-diethylphenyl)-N-(methoxymethyl)acetamide

Synonyms: 2-Chloro-2′,6′-diethyl-N-(methoxymethyl)-acetanilide
Methachlor

Molecular Formula: $C_{14}H_{20}ClNO_2$

Structure:



Chemical Properties

Molecular Weight: 269.90

Vapor Pressure: 2.2×10^{-5} mm at 25°C

Boiling Point: 100°C

Density:

Octanol/Water Partition Coefficient:

Physical State:

Vapor Density:

Melting Point:

Solubility: 140 ppm H_2O

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 20×10^6 lbs.

Consumption: 20×10^6 lbs.

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 20.2

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1200 mg/kg	rat	oral
	3000 mg/kg	mammal	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Aldrin

CHEMICAL NAME

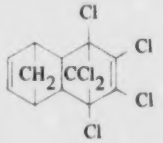
CAS Number: 309-00-2

Chemical Name: 1,2,3,4,10,10-Hexachloro-1,4,4a,5,8,8a-hexahydro-endo,exo-1,4:5,8-dimethanonaphthalene

Synonyms: Octalene
Aldrine
Compound 118

Molecular Formula: $C_{12}H_8Cl_6$

Structure:



Chemical Properties

Molecular Weight: 364.82

Vapor Pressure: 2.31×10^{-5} Torrs at 20°C

Boiling Point:

Density:

Octanol/Water Partition Coefficient: 5.00

Physical State: Solid

Vapor Density:

Melting Point: 104°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Can be degraded anaerobically
Aldrin → dieldrin in the environment

Safety Hazard:

Aldrin

PRODUCTION DATA

Annual U.S. Production: 25 x 10^6 lbs.

Consumption: 25 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 25.3 (1972)

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	55 mg/kg	rat	oral
	200 mg/kg	rat	skin
	39 mg/kg	rat	oral
	98 mg/kg	rat	skin
	10 mg/kg	chicken	oral
	7 mg/kg	wild bird	oral
LD_{Lo}	15 mg/kg	rat	skin
	63 mg/kg	mouse	intraperitoneal
	95 mg/kg	dog	unknown

Non-lethal Acute Effects:

- Irritability
- Convulsions
- Liver damage

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Neoplastic effects

TD_{Lo}: 440 mg/kg (52 weeks)–mouse, oral

Mutagenicity:

Teratogenicity:

TLV: 0.25 mg/m^3 (skin)

Other Chronic Effects:

Allyl alcohol

CHEMICAL NAME

CAS Number: 107-18-6

Chemical Name: Allyl alcohol

Synonyms: 2-Propen-1-ol
Vinyl carbinol

Molecular Formula: C_3H_6O

Structure: $CH_2 = CH - CH_2OH$

Chemical Properties

Molecular Weight: 58.08

Physical State: Liquid

Vapor Pressure: 25.6 mm at 25°C

Vapor Density: 2.00

Boiling Point: 97°C

Melting Point: -129°C

Density: 0.8540 at 20°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient: 0.13

Environmental Persistence

BOD: 9.1% of theoretical

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:

Fire–dangerous
Explosion–moderate
Disaster hazard–dangerous–toxic fumes

Allyl alcohol

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	42 mg/kg	rat	intraperitoneal
	96 mg/kg	mouse	oral
	42 mg/kg	mouse	intraperitoneal
LD_{Lo}	69 mg/kg	rat	oral
	43 mg/kg	dog	oral
	53 mg/kg	rabbit	oral
	53 mg/kg	rabbit	skin
	45 mg/kg	rabbit	parenteral
LC_{50}	165 ppm (4 hours)	rat	inhalation
LC_{Lo}	1000 ppm (4 hours)	monkey	inhalation
	1000 ppm (4 hours)	rabbit	inhalation

Non-lethal Acute Effects:

Irritant effects:

TC_{Lo}	25 ppm	human	inhalation

Eyes and skin irritated

Respiratory tract irritated

Damage to kidney and liver

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 2 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 2 ppm (skin)

Other Chronic Effects:

Allyl chloride

CHEMICAL NAME

CAS Number: 107-05-1

Chemical Name: 3-Chloropropene

Synonyms:		
	3-Chloroprene	1-Chloro-2-propene
	AC	3-Chloropropylene
	Chlorallylene	2-Chloropropylene

Molecular Formula: C_3H_5Cl

Structure: $CH_2 = CH - CH_2 Cl$

Chemical Properties

Molecular Weight: 76.53	**Physical State:** Liquid
Vapor Pressure: 359 mm at 25°C	**Vapor Density:** 2.64
Boiling Point: 44.6°C	**Melting Point:** −134.5°C
Density: 0.938 at 20°C/4°C	**Solubility:** Soluble (3.3 gm/l H_2O)
Octanol/Water Partition Coefficient:	

Environmental Persistence

BOD:

Atmospheric Reactivity: Unreactive to O_2
Reacts vigorously with oxidizing materials
Reactive with O_3, $t_{1/2}$ = 9 hours, yielding formaldehyde and 2-chloroacetaldehyde
Reactive with OH, $t_{1/2}$ = 21 hours, yielding 2-chloroacetaldehyde

Safety Hazard: Fire–highly dangerous
Explosion–moderate

Allyl chloride

PRODUCTION DATA

Annual U.S. Production: 295.0 x 10^6 lbs.

Consumption: 295.0 x 10^6 lbs.

Fraction of Dispersion: 0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 4.4 (1972)

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	155 mg/kg	mouse	intraperitoneal
	7150 mg/kg	dog	intravenous
	2200 mg/kg	rabbit	skin
LD_{Lo}	64 mg/kg	rat	oral
LC_{Lo}	290 ppm (8 hours)	rat	inhalation
	6360 ppm	guinea pig	inhalation

Pulmonary hemorrhage

Chronic Toxicity

U.S. Occupational Standard: TWA: 1 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity: TLV: 1 ppm

Other Chronic Effects: Irritation of eyes, nose, and throat
Degeneration of liver and kidney

Allylene

CHEMICAL NAME

CAS Number: 74-99-7

Chemical Name: Propyne

Synonyms: Allylene
Methylacetylene
Propine

Molecular Formula: C_3H_4

Structure: $CH_3 - C \equiv CH$

Chemical Properties

Molecular Weight: 40.07

Vapor Pressure: 3876 mm at 20°C

Boiling Point: -23.2°C at 760 mm

Density: 0.7062 at -50°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Gas

Vapor Density: 1.38

Melting Point: -101.5°C

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts violently with oxidizing materials

Safety Hazard:
Fire–dangerous
Explosion–moderate

Allylene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**

Non-lethal Acute Effects:

Anesthetic
Asphyxiant in high concentrations

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Allyl naphthalene

CHEMICAL NAME

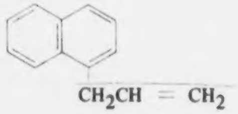
CAS Number: 2489-86-3

Chemical Name: 1-Allylnaphthalene

Synonyms: 3-α-Naphthylpropene

Molecular Formula: $C_{13}H_{12}$

Structure:



Chemical Properties

Molecular Weight: 168.24

Vapor Pressure:

Boiling Point: 265 to 267°C

Density: 1.0228 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point:

Solubility:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Allyl naphthalene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Amiben

CHEMICAL NAME

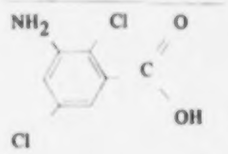
CAS Number: 133-90-4

Chemical Name: 3-Amino-2,5-dichlorobenzoic acid

Synonyms: 2,5-Dichloro-3-aminobenzoic acid

Molecular Formula: $C_7H_5Cl_2NO_2$

Structure:



Chemical Properties

Molecular Weight: 205.96

Vapor Pressure: Negligible at 25°C

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 201°C

Solubility: 700 ppm (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous–toxic fumes

PRODUCTION DATA

Annual U.S. Production: 20 x 10^6 lbs.

Consumption: 20 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 20.2

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	5620 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

p-Aminobenzoic acid

CHEMICAL NAME

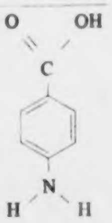
CAS Number: 150-13-0

Chemical Name: p-Aminobenzoic acid

Synonyms: PABA
Paraminol

Molecular Formula: $C_7H_7NO_2$

Structure:



Chemical Properties

Molecular Weight:	137.14	**Physical State:**	Solid
Vapor Pressure:		**Vapor Density:**	
Boiling Point:		**Melting Point:**	188 to 189°C
Density:	1.374 at 25°C/4°C	**Solubility:**	Soluble (hot H_2O)
Octanol/Water Partition Coefficient:	0.89		

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

p-Aminobenzoic acid

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	2850 mg/kg	mouse	oral
	1830 mg/kg	rabbit	oral
	2000 mg/kg	rabbit	intervenous
LD_{Lo}	6000 mg/kg	rat	oral
	1000 mg/kg	dog	oral

Non-lethal Acute Effects:

Methemoglobinemia
Hepatitis

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

p-Aminobiphenyl

CHEMICAL NAME

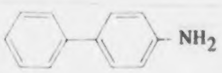
CAS Number: 92-67-1

Chemical Name: 4-Biphenylamine

Synonyms: 4-Aminobiphenyl
Xenylamine
p-Biphenylamine

Molecular Formula: $C_{12}H_{11}N$

Structure:



Chemical Properties

Molecular Weight:	169.23	**Physical State:**	Solid
Vapor Pressure:		**Vapor Density:**	
Boiling Point:	302°C	**Melting Point:**	53 to 54°C
Density:	1.160 at 20°C/20°C	**Solubility:**	Slightly (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–moderate–toxic fumes

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	500 mg/kg	rat	oral
LD_{Lo}	250 mg/kg	mouse	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard: (air) Carcinogen

Carcinogenicity:

TD_{Lo}	5200 mg/kg (52 weeks)	rat	oral
	4 g/kg	rat	subcutaneous
	140 mg/kg (7 days)	mouse	oral
	216 mg/kg (3 days)	mouse	subcutaneous
	680 mg/kg (3 years)	dog	oral

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Aminoethylethanolamine

CHEMICAL NAME

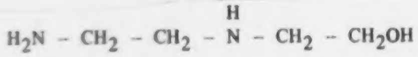
CAS Number: 111-41-1

Chemical Name: 2[(2-Aminoethyl)amino] ethanol

Synonyms: (2-Hydroxyethyl)-ethylenediamine
N-Aminoethylethanolamine

Molecular Formula: $C_4H_{12}N_2O$

Structure:



$$H_2N - CH_2 - CH_2 - \overset{H}{N} - CH_2 - CH_2OH$$

Chemical Properties

Molecular Weight: 104.16

Vapor Pressure: <0.01 mm at 20°C

Boiling Point: 243.7°C at 760 mm

Density: 0.9556 at 25°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 3.59

Melting Point:

Solubility: Very soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–moderate

Aminoethylethanolamine

PRODUCTION DATA

Annual U.S. Production: 13.5 x 10^6 lbs.

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3000 mg/kg	rat	oral
	1800 mg/kg	guinea pig	skin

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Amyl acetate

CHEMICAL NAME

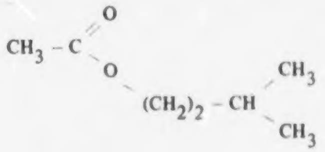
CAS Number: 628-63-7

Chemical Name: Acetic acid, pentyl ester

Synonyms:
- Isoamyl acetate
- Banana oil
- Isopentyl acetate
- Acetic acid
- Amylacetic ester

Molecular Formula: $C_7H_{14}O_2$

Structure:



Chemical Properties

Molecular Weight: 130.2

Vapor Pressure: 9.43 mm at 25°C

Boiling Point: 142.0°C

Density: 0.876 at 15°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 4.49

Melting Point:

Solubility: Slight (H_2O)

Environmental Persistence

BOD: 38% of theoretical

Atmospheric Reactivity: Reacts with reducing material

Safety Hazard: Fire–dangerous
Explosion–moderate

Amyl acetate

PRODUCTION DATA

Annual U.S. Production: 7.6 x 10^6 lbs. (1964)

Consumption:

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 7.6

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	7400 mg/kg	rabbit	oral
LD_{Lo}	1500 mg/kg	rat	intraperitoneal
LC_{Lo}	5200 ppm		

Non-lethal Acute Effects:

Irritant effects–TC_{Lo} 188 ppm (30 minutes) human inhalation
Inhalation–1000 ppm (30 minutes) causes headache, fatigue, chest oppression
Irritant–eyes and mucous membranes of nose and throat

Chronic Toxicity

U.S. Occupational Standard: TWA: 125 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:

Amyl alcohol

CHEMICAL NAME

CAS Number: 71-41-0

Chemical Name: Pentyl alcohol

Synonyms:
n-Amyl alcohol
1-Pentanol
Primary amyl alcohol
Butyl carbinol

Molecular Formula: $C_5H_{12}O$

Structure: $CH_3 - CH_2 - CH_2 - CH_2 - CH_2OH$

Chemical Properties

Molecular Weight: 88.15

Vapor Pressure: 3.16 mm at 25°C

Boiling Point: 137.3°C at 748 mm

Density: 0.8144 at 20°C/4°C

Octanol/Water Partition Coefficient: 1.56

Physical State: Liquid

Vapor Density: 3.04

Melting Point: -79°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD: 84% of theoretical

Atmospheric Reactivity:

Safety Hazard:
Fire–moderate
Explosion–moderate

Amyl alcohol

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	3030 mg/kg	rat	oral
	200 mg/kg	mouse	oral
LD_{Lo}	490 mg/kg	rat	intraperitoneal
	1390 mg/kg	dog	oral

Non-lethal Acute Effects:

Vapor irritant to eyes and upper respiratory tract

Following ingestion:

- Headache
- Nausea and vomiting
- Delirium
- Methemoglobin formation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:

Amylamines

CHEMICAL NAME

CAS Number: 110-58-7

Chemical Name: Pentylamine

Synonyms: Amylamine (mixed isomers)
Aminopentane

Molecular Formula: $C_5H_{13}N$

Structure: $CH_3(CH_2)_3CH_2NH_2$ (1 – amyl amine)

Chemical Properties (1-amylamine)

Molecular Weight: 87.17

Vapor Pressure:

Boiling Point: 104.4°C at 760 mm

Density: 0.7547 at 20°C/4°C

Octanol/Water Partition Coefficient: 1.05

Physical State: Liquid

Vapor Density: 3.01

Melting Point: -55°C

Solubility: Infinite (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous

Amylamines

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
(Mixed isomers)			
LD_{50}	470 mg/kg	rat	oral
	1120 mg/kg	rabbit	skin
LC_{Lo}	2000 ppm (4 hours)	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:
Strong irritant

Amyl chloride

CHEMICAL NAME

CAS Number: 543-59-7

Chemical Name: 1-Chloropentane

Synonyms: n-Amylchloride
Pentylchloride

Molecular Formula: $C_5H_{11}Cl$

Structure: $CH_3(CH_2)_3CH_2Cl$

Chemical Properties

Molecular Weight: 106.6

Physical State: Liquid

Vapor Pressure: 10 mm at 25°C

Vapor Density: 3.67

Boiling Point: 107.8°C at 760 mm

Melting Point: -99°C

Density: 0.8818 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:

Fire–dangerous
Explosion–explosive if mixed with air
Disaster hazard–dangerous–emits toxic fumes (phosgene)

Amyl chloride

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**

Non-lethal Acute Effects:
Narcotic
Local irritant

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Amylene

CHEMICAL NAME

CAS Number: 109-67-1

Chemical Name: 1-Pentene

Synonyms: Amylene
Propyl ethylene

Molecular Formula: C_5H_{10}

Structure: $CH_3CH_2CH_2CH = CH_2$

Chemical Properties

Molecular Weight: 70.14

Vapor Pressure: 858.0 mm at 25°C

Boiling Point: 29.968°C at 760 mm

Density: 0.6405 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Gas-liquid

Vapor Density: 2.42

Melting Point: -138°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous toxic fumes

Amylene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Non-lethal Acute Effects:

Narcotic
Asphyxiant

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Amyl ether

CHEMICAL NAME

CAS Number: 693-65-2

Chemical Name: Pentyl ether

Synonyms: Amyl ether
Amyl oxide
Diamyl ether

Molecular Formula: $C_{10}H_{22}O$

Structure: $CH_3(CH_2)_4 - O - (CH_2)_4 - CH_3$

Chemical Properties

Molecular Weight: 158.29

Vapor Pressure:

Boiling Point: 190°C at 760 mm

Density: 0.7833 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 5.46

Melting Point: -69°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–moderate

Amyl ether

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Amyl mercaptan

CHEMICAL NAME

CAS Number: 110-66-7

Chemical Name: 1-Pentane thiol

Synonyms:
Amyl mercaptan
Amyl hydrosulfide
Amy sulfhydrate
Amyl thio alcohol
n-Thioamyl alcohol

Molecular Formula: $C_5H_{12}S$

Structure: $CH_3CH_2CH_2CH_2CH_2SH$

Chemical Properties

Molecular Weight: 104.22

Vapor Pressure: 13.8 mm at 25°C

Boiling Point: 112.9°C at 760 mm

Density: 0.8327 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 3.59

Melting Point: -169°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous

Amyl mercaptan

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LC_{Lo}	2000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Irritant to eyes and skin

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Aniline

CHEMICAL NAME

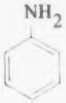
CAS Number: 62-53-3

Chemical Name: Aniline

Synonyms:
Benzenamine
Aminobenzine
Aminophen
Benzamine
Phylamine
Aniline oil

Molecular Formula: C_6H_7N

Structure:



Chemical Properties

Molecular Weight: 93.12

Physical State: Liquid

Vapor Pressure: 0.67 mm at 25°C

Vapor Density: 3.22

Boiling Point: 184°C

Melting Point: –6.3

Density: 1.02173 at 20°C/4°C

Solubility: Soluble, (36.5 gm/l of H_2O)

Octanol/Water Partition Coefficient: 1.24

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials
Photochemically degraded to n-methylaniline, N,N-dimethylaniline, acetanilide, phenol, and isomeric hydroxyanilines

Safety Hazard: Fire–moderate
Disaster hazard–dangerous, toxic fumes

Aniline

PRODUCTION DATA

Annual U.S. Production: 551.2 x 10^6 lbs. (1974)

Consumption: 480 x 10^6 lbs.

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 6.15

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	440 mg/kg	rat	oral
	1400 mg/kg	rat	skin
	420 mg/kg	rat	intraperitoneal
	820 mg/kg	rabbit	skin
	64 mg/kg	rabbit	intravenous
	1290 mg/kg	guinea pig	skin
LD_{Lo}	350 mg/kg	human	oral
	357 mg/kg	human	unreported
	480 mg/kg	mouse	subcutaneous
	1540 mg/kg	dog	skin
	1750 mg/kg	cat	oral
	1540 mg/kg	cat	skin
	200 mg/kg	rabbit	intraperitoneal
	1000 mg/kg	rabbit	subcutaneous
	1750 mg/kg	guinea pig	skin
LC_{50}	175 ppm (7 hours)	mouse	inhalation
LC_{Lo}	250 ppm (4 hours)	rat	inhalation
	180 ppm (8 hours)	cat	inhalation

Chronic Toxicity

U.S. Occupational Standard: TWA: 5 ppm

Carcinogenicity: Neoplastic effects–papillomas and benign bladder tumors

Mutagenicity:

Teratogenicity:

TLV: 5 ppm (skin)
Odor perception: 0.23 ppm

Other Chronic Effects:
Nephrosis
Blood effects
Enzyme and hormone effects

Aniline hydrochloride

CHEMICAL NAME

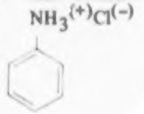
CAS Number: 142-04-1

Chemical Name: Aniline hydrochloride

Synonyms: Aniline chloride
Benzenamine hydrochloride
Aniline salt

Molecular Formula: $C_6H_7N \cdot HCl$

Structure:



Chemical Properties

Molecular Weight: 129.60

Physical State: Solid

Vapor Pressure:

Vapor Density: 1.22 at 4°C

Boiling Point: 245°C at 760 mm

Melting Point: 198°C

Density: 1.2215 at 4°C

Solubility: Very soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–slight
Disaster hazard–dangerous if heated with acid; aniline and chlorine fumes

Aniline hydrochloride

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1072 mg/kg	rat	oral
	841 mg/kg	mouse	oral
	750 mg/kg	mouse	intraperitoneal
LD_{Lo}	500 mg/kg	rat	intraperitoneal

Non-lethal Acute Effects:

Depression of CNS
Methemoglobinemia
Hemolysis
Stimulation of bone marrow
Liver damage

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Anisidine (o and p)

CHEMICAL NAME

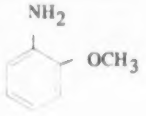
CAS Number: 104-97-9(p); 90-04-0(o)

Chemical Name: p-Anisidine; o-Anisidine

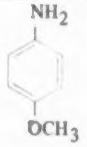
Synonyms:
o-Methoxyaniline
o-Aminoanisole
p-Methoxyaniline
p-Aminoanisole
1-Amino-4-methoxybenzene

Molecular Formula: C_7H_9NO

Structure:



(o)



(p)

Chemical Properties

Molecular Weight: 123.16

Vapor Pressure: 1 mm at 61°C

Boiling Point: 224°C at 760 mm (o)
243°C at 760 mm (p)

Density: 1.0923 at 20°C/4°C (o)
1.071 at 57°C/4°C (p)

Octanol/Water Partition Coefficient: 1.65

Physical State: Liquid

Vapor Density:

Melting Point: 6.22°C (o)
57.2°C (p)

Solubility: Soluble (H_2O) (p)
Slightly soluble (H_2O) (o)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous, toxic fumes

Anisidine (o and p)

PRODUCTION DATA

Annual U.S. Production: 2.3 x 10^6 lbs. (total, 1967)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
(p-Anisidine)			
LD_{50}	1400 mg/kg	rat	oral
	1400 mg/kg	rat	intraperitoneal

Non-lethal Acute Effects:
Irritant to skin

Chronic Toxicity

U.S. Occupational Standard: (o and p isomers) (air) TWA 0.5 mg/m^3

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 0.5 mg/m^3 (skin)

Other Chronic Effects:

Anisole

CHEMICAL NAME

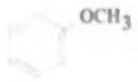
CAS Number: 100-66-3

Chemical Name: Anisole

Synonyms:
Methoxy benzene
Methylphenyl ether
Phenylmethyl ether

Molecular Formula: C_7H_8O

Structure:



Chemical Properties

Molecular Weight: 108.15

Physical State: Liquid

Vapor Pressure: 10 mm at 42.2°C

Vapor Density: 3.72

Boiling Point: 155°C

Melting Point: -37.5°C

Density: 0.9961 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient: 2.27

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts towards oxidizing materials

Safety Hazard:
Fire–moderate

Anisole

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	3700 mg/kg	rat	oral
	2800 mg/kg	mouse	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Anthranilic acid

CHEMICAL NAME

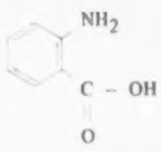
CAS Number: 118-92-3

Chemical Name: Anthranilic acid

Synonyms: O-Aminobenzoic acid
2-Aminobenzoic acid

Molecular Formula: $C_7H_7NO_2$

Structure:



Chemical Properties

Molecular Weight: 137.14

Vapor Pressure:

Boiling Point: Sublimes

Density: 1.412 at 20°C

Octanol/Water Partition Coefficient: 1.73

Physical State: Solid

Vapor Density:

Melting Point: 146 to 147°C

Solubility: Soluble (H_2O)
Very soluble (hot H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–slight

Anthranilic acid

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	4620 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Neoplastic effects:			
TD_{Lo}	16 gm/kg (24 weeks)	rat	oral

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Anthraquinone

CHEMICAL NAME

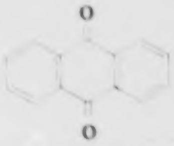
CAS Number: 84-65-1

Chemical Name: Anthraquinone

Synonyms: 9,10-Dihydro-9,10-dioxoanthracenedione

Molecular Formula: $C_{14}H_8O_2$

Structure:



Chemical Properties

Molecular Weight:	208.23	**Physical State:**	Solid
Vapor Pressure:	1 mm at 190°C	**Vapor Density:**	7.16
Boiling Point:	379.8°C at 760 mm	**Melting Point:**	286°C (sublimes)
Density:	1.438 at 4°C	**Solubility:**	Insoluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire - slight

Anthraquinone

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**

Non-lethal Acute Effects:
Weak sensitizer–dermatitis

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:
Neoplastic effects:

TD_{Lo}	90 gm/kg (90 days)	rat	oral

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Auramine

CHEMICAL NAME

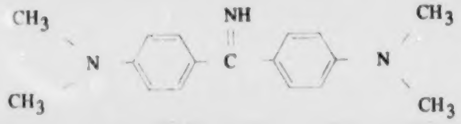
CAS Number: 492-80-8

Chemical Name: 4,4'-Carbonimidoylbis[N,N-dimethyl] benzenamine

Synonyms: 4,4'-(Imidocarbonyl)bis(N,N-dimethyl)aniline
Auramine
Bis(p-dimethylamine-phenyl)methyleneimine
Apyonin

Molecular Formula: $C_{17}H_{21}N_3$

Structure:



Chemical Properties

Molecular Weight: 267.38

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 136°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Auramine

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**

Non-lethal Acute Effects:
Dermatitis

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Neoplastic effects:			
TD_{Lo}	37 gm/kg (87 weeks continuous)	rat	oral
	2625 mg/kg (21 weeks intermittent)	rat	subcutaneous
Carcinogenic effect:			
TD_{Lo}	29 gm/kg (52 weeks continuous)	mouse	oral

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Azodrin

CHEMICAL NAME

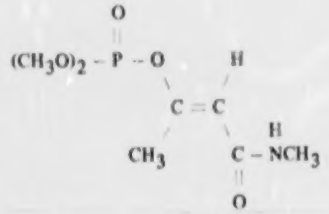
CAS Number: 919-44-8

Chemical Name: Phosphoric acid, (Z)dimethyl-1-methyl-3(methylamino)-2-oxo-1-propenyl ester

Synonyms:
Phosphoric acid, dimethyl ester with (E)-hydroxyl-N-methylcrotonamide
Dimethyl phosphate of 3-hydroxy-N-methyl-cis-crotonamide
Monocroptophos
O,O-dimethyl-O-(2-methylcarbamoyl-1-methyl-vinyl)-phosphate

Molecular Formula: $C_7H_{14}NO_5P$

Structure:



Chemical Properties

Molecular Weight: 223.19

Vapor Pressure:

Boiling Point: 125°C at 760 mm

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point:

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–dangerous
Disaster hazard–moderate–toxic fumes

PRODUCTION DATA

Annual U.S. Production: 5×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 5

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2 mg/kg	rat	oral
	2 mg/kg	mouse	oral
	7 mg/kg	dog	oral
	11 mg/kg	rabbit	oral
	107 mg/kg	rabbit	skin

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Banvel D

CHEMICAL NAME

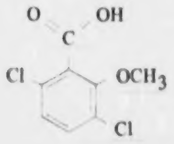
CAS Number: 1918-00-9

Chemical Name: 3,6-Dichloro-2-methoxybenzoic acid

Synonyms: 3,6-Dichloro-o-anisic acid
Dicamba

Molecular Formula: $C_8H_6Cl_2O_3$

Structure:



Chemical Properties

Molecular Weight:	221.04	**Physical State:**	Solid
Vapor Pressure:		**Vapor Density:**	
Boiling Point:		**Melting Point:**	114 to 116°C
Density:		**Solubility:**	Slightly soluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 2×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 2

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1040 mg/kg	rat	oral
	1190 mg/kg	mouse	oral
	2000 mg/kg	rabbit	oral
	3000 mg/kg	guinea pig	oral
	1000 mg/kg	mammal	unknown

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Banvel T

CHEMICAL NAME

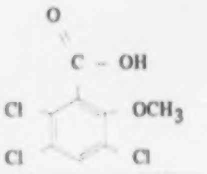
CAS Number: 2307-49-5

Chemical Name: 3,5,6-Trichloro-o-anisic acid

Synonyms: Tricamba
2-Methoxy-3,5,6-trichlorobenzoic acid
3,5,6-Trichloro-2-methoxybenzoic acid

Molecular Formula: $C_8H_5O_3Cl_3$

Structure:



Chemical Properties

Molecular Weight: 255.4

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 137 to 139°C

Solubility: Slightly soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	300 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Benzaldehyde

CHEMICAL NAME

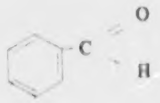
CAS Number: 100-52-7

Chemical Name: Benzaldehyde

Synonyms: Benzoic aldehyde
Artificial almond oil
Benzenecarbonal

Molecular Formula: C_7H_6O

Structure:



Chemical Properties

Molecular Weight: 106.12

Vapor Pressure: 1 mm at 26.2°C

Boiling Point: 179.0°C

Density: 1.050 at 15°C/5°C

Octanol/Water Partition Coefficient: 2.41

Physical State: Liquid

Vapor Density: 3.65

Melting Point: -26°C

Solubility: slight (H_2O)

Environmental Persistence

BOD: 50% of theoretical after 10 days

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–slight

PRODUCTION DATA

Annual U.S. Production: 3.4 x 10^6 lbs. (1968)

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1300 mg/kg	rat	oral
	1000 mg/kg	guinea pig	oral
LD_{Lo}	5000 mg/kg	rat	subcutaneous

Non-lethal Acute Effects:

Dermatitis
Narcosis

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Benzamide

CHEMICAL NAME

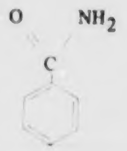
CAS Number: 55-21-0

Chemical Name: Benzamide

Synonyms: Benzoylamide
Benzoic acid, amide

Molecular Formula: C_7H_7NO

Structure:



Chemical Properties

Molecular Weight: 121.14

Vapor Pressure:

Boiling Point: 290°C

Density: 1.0792 at 130°C/4°C

Octanol/Water Partition Coefficient: 0.96

Physical State: Solid

Vapor Density:

Melting Point: 132.5°C

Solubility: Slightly (H_2O)
Very soluble (hot H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1160 mg/kg	mouse	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Benzene

CHEMICAL NAME

CAS Number: 71-43-2

Chemical Name: Benzene

Synonyms: Benzol
Phenylhydride
Coal naptha

Molecular Formula: C_6H_6

Structure:

Chemical Properties

Molecular Weight: 78.11

Vapor Pressure: 95.9 mm at 25°C

Boiling Point: 80.1°C at 760 mm

Density: 0.8787 at 20°C/4°C

Octanol/Water Partition Coefficient: 2.28

Physical State: Liquid

Vapor Density: 2.77

Melting Point: 5.5°C

Solubility: Slightly (1.79 gm/l of H_2O)

Environmental Persistence

BOD: 1.9% theoretical

Atmospheric Reactivity:
Activity toward O_2: slowly reacts with oxidizing materials
Activity toward OH: $t_{1/2}$ = 3 days
Photochemical Degradation: Not photoreactive; is biodegradable; found in air at 0.015-0.057 ppm

Safety Hazard:

Benzene

PRODUCTION DATA

Annual U.S. Production: 11,120 x 10^6 lbs. (1974)

Consumption: 1,562.8 x 10^6 lbs.

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 183.6

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	3800 mg/kg	rat	oral
	4700 mg/kg	mouse	oral
	468 mg/kg	mouse	intraperitoneal
	1150 mg/kg	rat	intraperitoneal
LD_{Lo}	2000 mg/kg	dog	oral
	530 mg/kg	guinea pig	intraperitoneal
	1400 mg/kg	frog	subcutaneous

Non-lethal Acute Effects:

Blood effects–TC_{Lo}:		human	inhalation

Aplastic anemia
Local irritant–erythemia, burning of skin
Narcotic action on CNS
Euphoria

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 10 ppm

Carcinogenicity: TD_{Lo} 1232 mg/kg (52 weeks) mouse skin
Implicated in human leukemia, sarcoma

Mutagenicity: Positive pulmonary adenomas
Bone marrow cell breaks

Teratogenicity: No information

TLV: 10 ppm

Other Chronic Effects: Estrus cycle disorder
Liver, kidney and lung damage
Hormone alteration
Bone marrow hyperplasia

Benzenedisulfonic acid

CHEMICAL NAME

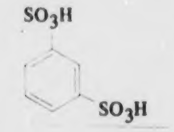
CAS Number: 30496-93-6

Chemical Name: m-Benzene disulfonic acid

Synonyms: MBDSA

Molecular Formula: $C_6H_6O_6S_2$

Structure:



Chemical Properties

Molecular Weight:	238.23	**Physical State:**	Solid
Vapor Pressure:		**Vapor Density:**	
Boiling Point:		**Melting Point:**	
Density:		**Solubility:**	Soluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Benzenedisulfonic acid

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**

Non-lethal Acute Effects:
Irritant

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Benzenesulfonic acid

CHEMICAL NAME

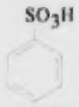
CAS Number: 98-11-3

Chemical Name: Benzene sulfonic acid

Synonyms: Phenyl sulfonic acid

Molecular Formula: $C_6H_6O_3S$

Structure:



Chemical Properties

Molecular Weight: 158.12

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient: -2.25

Physical State: Solid

Vapor Density:

Melting Point: 65 to 66°C (anhydrous)

Solubility: Very soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Benzenesulfonic acid

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	2050 mg/kg	rat	oral

Non-lethal Acute Effects:
Irritant

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Benzidine

CHEMICAL NAME

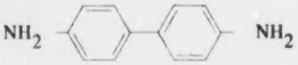
CAS Number: 92-87-5

Chemical Name: Benzidine

Synonyms:
[1,1'-Biphenyl]-4,4'-diamine
p-Diaminodiphenyl
4,4'-Biphenyldiamine
4,4'-Diaminodiphenyl
4,4'-Diphenylenediamine

Molecular Formula: $C_{12}H_{12}N_2$

Structure:



Chemical Properties

Molecular Weight: 184.24

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 401.7°C

Melting Point: 122 and 125°C–unstable
128°C–stable

Density: 1.250 at 20°C/4°C

Solubility: Slightly soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD: 1.9 for 20 days at 20°C

Atmospheric Reactivity:
Reacts rapidly with RO_2 ($t_{1/2}$ = 4 days)
O_3 ($t_{1/2}$ = 1 day)
OH ($t_{1/2}$ = 1 day)

Safety Hazard:

Benzidine

PRODUCTION DATA

Annual U.S. Production: 10.4 x 10^6 lbs (1972)

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): .02

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	309 mg/kg	rat	oral
	214 mg/kg	mouse	oral
LD_{Lo}	200 mg/kg	dog	oral
	400 mg/kg	dog	subcutaneous

Non-lethal Acute Effects:

Bone marrow depression
Liver and kidney damage
Blood hemolysis
Epicardial petechial hemorrhage

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

TD_{Lo}	4500 mg/kg (30 days)	rat	oral
	2100 mg/kg (35 weeks)	rat	subcutaneous
	8 gm/kg (35 weeks)	mouse	subcutaneous
	75 gm/kg (3 years)	hamster	oral
TC_{Lo}	10 mg/m^3 (56 weeks)	rat	inhalation
	18 mg/m^3 (13 years)	human	inhalation

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Benzil

CHEMICAL NAME

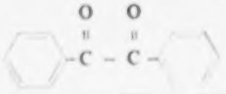
CAS Number: 134-81-6

Chemical Name: Benzil

Synonyms: Dibenzoyl
Diphenyl-ethanedione
Diphenylglyoxal

Molecular Formula: $C_{14}H_{10}O_2$

Structure:



Chemical Properties

Molecular Weight: 210.2

Vapor Pressure: 1 mm at 128.4°C

Boiling Point: 346 to 348°C (decomposes)

Density: 1.084 at 102°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 95°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	2710 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Benzilic acid

CHEMICAL NAME

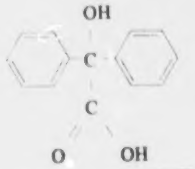
CAS Number: 76-93-7

Chemical Name: Benzilic acid

Synonyms: Diphenyl glycolic acid
Diphenyl hydroxyacetic acid
α-Hydroxy-α-phenylbenzene acetic acid

Molecular Formula: $C_{14}H_{12}O_3$

Structure:



Chemical Properties

Molecular Weight: 228.24

Vapor Pressure:

Boiling Point: 180°C (decomposes)

Density:

Octanol/Water Partition Coefficient: 2.32

Physical State: Solid

Vapor Density:

Melting Point: 148 to 151°C

Solubility: Slightly soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire – slight

Benzilic acid

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Benzoic acid

CHEMICAL NAME

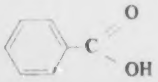
CAS Number: 65-85-0

Chemical Name: Benzoic Acid

Synonyms: Phenyl formic acid
Benzene carboxylic acid
Carboxybenzene

Molecular Formula: $C_7H_6O_2$

Structure:



Chemical Properties

Molecular Weight: 122.12

Physical State: Solid

Vapor Pressure: 1 mm at 96.0°C

Vapor Density: 4.21

Boiling Point: 249°C

Melting Point: 122.4°C

Density: 1.2659 15°C/4°C

Solubility: Slightly (H_2O)

Octanol/Water Partition Coefficient: 2.00

Environmental Persistence

BOD: 46% of theoretical after 10 days

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–slight

PRODUCTION DATA

Annual U.S. Production: 79 x 10^6 lbs. (1974)

Consumption: 70 x 10^6 lbs. (1975)
(excludes phenol production)
ca. 90 x 10^6 lbs.
(phenol production)

Fraction of Dispersion: 0.01

Release Rate (million lbs/yr):

Fraction of Production Lost: 0.015

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	3040 mg/kg	rat	oral
	2370 mg/kg	mouse	oral
	1460 mg/kg	mouse	intraperitoneal
Non-lethal Acute Effects:			
Skin effects–TD_{Lo}	6 mg/kg	human	skin
Gastrointestinal effects			

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Benzoin

CHEMICAL NAME

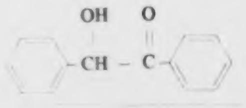
CAS Number: 119-53-9

Chemical Name: Benzoin

Synonyms: Phenyl α-hydroxybenzylketone
Phenylbenzoylcarbinol
Benzoylphenylcarbinol
2-Hydroxy-1,2-diphenylethanone

Molecular Formula: $C_{14}H_{12}O_2$

Structure:



Chemical Properties (dl mixture)

Molecular Weight: 212.24

Physical State: Solid

Vapor Pressure: 1 mm at 135.6°C

Vapor Density:

Boiling Point: 344°C at 768 mm

Melting Point: 137°C

Density: 1.310 at 20°C/4°C

Solubility: Slightly (hot H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire - slight

PRODUCTION DATA

Annual U.S. Production:	**Consumption:**
Fraction of Dispersion:	**Fraction of Production Lost:**
Release Rate (million lbs/yr):	

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity: TLV:

Other Chronic Effects:

Benzonitrile

CHEMICAL NAME

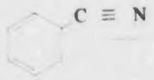
CAS Number: 100-47-0

Chemical Name: Benzonitrile

Synonyms: Phenyl cyanide
Benzoic acid, nitrile

Molecular Formula: C_7H_5N

Structure:



Chemical Properties

Molecular Weight:	103.13	**Physical State:**	Liquid
Vapor Pressure:	1 mm at 28.2°C	**Vapor Density:**	
Boiling Point:	190.7°C	**Melting Point:**	-13.1°C
Density:	1.246 at 20°C/4°C	**Solubility:**	Slightly (hot H_2O)
Octanol/Water Partition Coefficient:	1.56		

Environmental Persistence

BOD: 40% of theoretical

Atmospheric Reactivity:

Safety Hazard:

Benzonitrile

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1200 mg/kg	rat	skin
LD_{Lo}	720 mg/kg	rat	oral
	180 mg/kg	mouse	subcutaneous
LC_{Lo}	950 ppm (8 hours)	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Benzophenone

CHEMICAL NAME

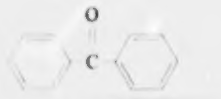
CAS Number: 119-61-9

Chemical Name: Benzophenone

Synonyms:
Phenyl ketone
Diphenyl ketone
Diphenyl methanone
Benzoylbenzene

Molecular Formula: $C_{13}H_{10}O$

Structure:



Chemical Properties

Molecular Weight: 182.21

Vapor Pressure: 1 mm at 108.2°C

Boiling Point: 305.9°C at 760 mm

Density: α form 1.0976 at 50°C/50°C

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 47.5°C (α)

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire – slight

Benzophenone

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Under test

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Benzoquinone

CHEMICAL NAME

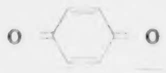
CAS Number: 106-51-4

Chemical Name: p-Benzoquinone

Synonyms:	Quinone Chinone	1,4-Benzoquinone Paraquinone

Molecular Formula: $C_6H_4O_2$

Structure:



Chemical Properties

Molecular Weight: 108.09	**Physical State:** Solid
Vapor Pressure:	**Vapor Density:**
Boiling Point: Sublimes	**Melting Point:** 115.7°C
Density: 1.318 at 20°C/4°C	**Solubility:** Soluble (H_2O)
Octanol/Water Partition Coefficient:	

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous–toxic fumes

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	130 mg/kg	rat	oral
	8500 mg/kg	mouse	intraperitoneal
	25 mg/kg	rat	intravenous
LC_{Lo}	320 mg/m^3	mouse	inhalation

Non-lethal Acute Effects:

Irritation of skin and mucous membranes
Necrosis, if in eyes
Kidney damage
Dermatitis

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

TD_{Lo}	2000 mg/kg (28 weeks)	mouse	skin

Mutagenicity:

Teratogenicity:

TLV: 0.1 mg/m^3

Other Chronic Effects:

Benzotrichloride

CHEMICAL NAME

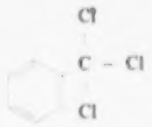
CAS Number: 98-07-7

Chemical Name: α,α,α-Trichlorotoluene

Synonyms: Phenylchloroform

Molecular Formula: $C_7H_5Cl_3$

Structure:



Chemical Properties

Molecular Weight: 195.48

Vapor Pressure: 1 mm at 45.8°C

Boiling Point: 220.6°C at 760 mm

Density: 1.38 at 15.5°C/15.5°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 6.77

Melting Point: –4.75°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Benzotrichloride

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{Lo}	2150 mg/kg	frog	unreported
LC_{Lo}	125 ppm (4 hours)	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Benzoyl chloride

CHEMICAL NAME

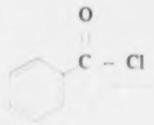
CAS Number: 98-88-4

Chemical Name: Benzoyl chloride

Synonyms: Benzene carbonyl chloride
α-Chlorobenzaldehyde

Molecular Formula: C_7H_5ClO

Structure:



Chemical Properties

Molecular Weight: 140.57

Physical State: Liquid

Vapor Pressure: 1 mm at 32.1°C

Vapor Density: 4.88

Boiling Point: 197.2°C at 760 mm

Melting Point: -0.5°C

Density: 1.2120 at 20°C/4°C

Solubility: Slightly (decomposes) (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD: 40% of theoretical

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous–fumes of phosgene

Benzoyl chloride

PRODUCTION DATA

Annual U.S. Production: Estimated as 16.8 x 10^6 lbs. (1975)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2460 mg/kg	rat	oral
	790 mg/kg	rabbit	skin
TC_{Lo}	16 ppm	human	inhalation

Non-lethal Acute Effects:

Irritant to skin, eyes, and mucous membranes
Lachrymatory

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Benzyl alcohol

CHEMICAL NAME

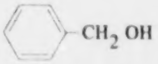
CAS Number: 100-51-6

Chemical Name: Benzyl alcohol

Synonyms:
Hydroxytoluene
Phenylcarbinol
α-Hydroxytoluene
Benzenemethanol

Molecular Formula: C_7H_8O

Structure:



Chemical Properties

Molecular Weight: 108.13

Vapor Pressure: 1 mm at 58.0°C

Boiling Point: 205.35°C at 760 mm

Density: 1.0419 at 20°C/4°C

Octanol/Water Partition Coefficient: 1.10

Physical State: Solid

Vapor Density: 3.72

Melting Point: -15.3°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD: 63% of theoretical

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–slight

Benzyl alcohol

PRODUCTION DATA

Annual U.S. Production: 10.4×10^6 lbs. (1972)

Consumption: 11.7×10^6 lbs. (1974)

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1230 mg/kg	rat	oral
	64 mg/kg	rat	intravenous
	1580 mg/kg	mouse	oral
	480 mg/kg	mouse	intravenous
	1940 mg/kg	rabbit	oral
	100 mg/kg	wild bird	oral
LD_{Lo}	400 mg/kg	rat	intraperitoneal
	50 mg/kg	dog	intravenous
	9 mg/kg	dog	parenteral
	400 mg/kg	guinea pig	intraperitoneal
LC_{50}	1000 pm (8 hours)		

Non-lethal Acute Effects:

Irritant–skin, mucous membranes

Headache, vertigo, nausea, vomiting, and diarrhea

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Benzylamine

CHEMICAL NAME

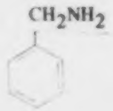
CAS Number: 100-46-9

Chemical Name: Benzenemethanamine

Synonyms: Aminotoluene

Molecular Formula: C_7H_9N

Structure:



Chemical Properties

Molecular Weight: 107.2

Vapor Pressure: 1 mm at 29°C

Boiling Point: 184.5°C

Density: 0.983 at 19°C/4°C

Octanol/Water Partition Coefficient: 1.14

Physical State: Liquid

Vapor Density:

Melting Point:

Solubility: Very soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–moderate–toxic fumes

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Benzylbenzene

CHEMICAL NAME

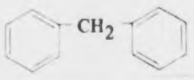
CAS Number: 101-81-5

Chemical Name: Diphenyl methane

Synonyms: Benzylbenzene
Ditan

Molecular Formula: $C_{13}H_{12}$

Structure:



Chemical Properties

Molecular Weight: 168.23

Vapor Pressure: 1 mm at 76.0°C

Boiling Point: 264.7°C at 760 mm

Density: 1.0056 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density: 5.79

Melting Point: 26.5°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire – slight

Benzylbenzene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{Lo}	5000 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Benzyl benzoate

CHEMICAL NAME

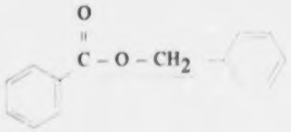
CAS Number: 120-51-4

Chemical Name: Benzoic acid, benzyl ester

Synonyms: Benzyl benzoate
Benzyl benzene carboxylate

Molecular Formula: $C_{14}H_{12}O_2$

Structure:



Chemical Properties

Molecular Weight:	212.25	**Physical State:**	Liquid
Vapor Pressure:	<10 mm at 25°C	**Vapor Density:**	7.3
Boiling Point:	323 to 324°C at 760 mm	**Melting Point:**	21°C
Density:	1.1121 at 25°C/4°C	**Solubility:**	Insoluble (H_2O)
Octanol/Water Partition Coefficient:	3.97		

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–slight

Benzyl benzoate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1700 mg/kg	rat	oral
	1400 mg/kg	mouse	oral
	2240 mg/kg	cat	oral
	1800 mg/kg	rabbit	oral
	1000 mg/kg	guinea pig	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Benzyl chloride

CHEMICAL NAME

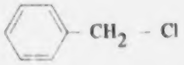
CAS Number: 100-44-7

Chemical Name: α-Chlorotoluene

Synonyms: α-Tolylchloride

Molecular Formula: C_7H_7Cl

Structure:



Chemical Properties

Molecular Weight: 126.5	**Physical State:** Liquid
Vapor Pressure: 1.4 mm at 25°C	**Vapor Density:** 4.36
Boiling Point: 179°C at 760 mm	**Melting Point:** -39°C
Density: 1.1026 at 18°C/4°C	**Solubility:** Insoluble (H_2O)
Octanol/Water Partition Coefficient:	

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing agents

Safety Hazard: Fire – moderate
Explosion – moderate (violent with metals)
Disaster hazard – dangerous fumes

Benzyl chloride

PRODUCTION DATA

Annual U.S. Production: 80.4 x 10^6 lbs. (1972)

Consumption: 90 x 10^6 lbs. (1974)

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1231 mg/kg	rat	oral
	1000 mg/kg	rat	subcutaneous
	1624 mg/kg	mouse	oral
Non-lethal Acute Effects:			
Unspecified effects:			
TC_{Lo}	16 ppm	human	inhalation
Irritant – intensely to eyes, skin, and mucous membranes			

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Neoplastic effects:			
TD_{Lo}	2100 mg/kg (51 weeks)	rat	subcutaneous

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects: CNS depression

Benzyldichloride

CHEMICAL NAME

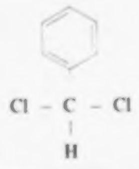
CAS Number: 98-87-3

Chemical Name: α,α-Dichlorotoluene

Synonyms:
Benzyl dichloride
Benzal chloride
Benzylidine chloride
(Dichloromethyl)-benzene

Molecular Formula: $C_7H_6Cl_2$

Structure:



Chemical Properties

Molecular Weight: 161.03

Vapor Pressure: <10 mm at 25°C

Boiling Point: 205.2°C at 760 mm

Density: 1.295 at 16°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point: -16.1°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Benzyldichloride

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	3249 mg/kg	rat	oral
	467 mg/kg	mouse	oral
LC_{50}	200 mg/m^3	mouse	inhalation

Non-lethal Acute Effects:
Irritant–strong lachrymator

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:
CNS despression

Bis (chloromethyl) ether

CHEMICAL NAME

CAS Number: 542-88-1

Chemical Name: Oxybis(chloromethane)

Synonyms:
Dichloromethyl ether
Dichlorinated methyloxide
BCME
1,1′-Dichlorodimethyl ether

Molecular Formula: $C_2H_4Cl_2O$

Structure: $ClCH_2 - O - CH_2Cl$

Chemical Properties

Molecular Weight: 114.96

Vapor Pressure:

Boiling Point: 104°C at 760 mm

Density: 1.328 at 15°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid (volatile)

Vapor Density: 4.0

Melting Point: −41.5°C

Solubility: Decomposes (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Bis (chloromethyl) ether

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	210 mg/kg	rat	oral
	280 mg/kg	rabbit	skin
TD_{Lo}	315 mg/kg (245 days, intermittent)	rat	subcutaneous
	11 gm/kg (47 weeks, intermittent)	mouse	skin

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Carcinogen, produces tumors

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Bisphenol A

CHEMICAL NAME

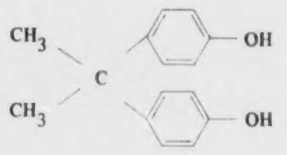
CAS Number: 80-05-7

Chemical Name: 4,4'-Isopropylidenediphenol

Synonyms: Bisphenol A
2,2-Bis (4-hydroxyphenyl) propane
4,4'-Isopropylidenediphenol

Molecular Formula: $C_{15}H_{16}O_2$

Structure:



Chemical Properties

Molecular Weight:	228.29	**Physical State:**	Solid
Vapor Pressure:	1 mm at 193°C	**Vapor Density:**	
Boiling Point:	250 to 252°C	**Melting Point:**	153°C
Density:		**Solubility:**	Insoluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 370.4 x 10^6 lbs. (1974)

Consumption: 370.4 x 10^6 lbs.

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	150 mg/kg	rat	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard: (air) TWA: 0.5 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:
(odorless)

Other Chronic Effects:

Bromacil

CHEMICAL NAME

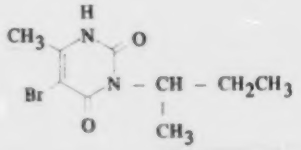
CAS Number: 314-42-1

Chemical Name: 5-Bromo-3-sec butyl-6-methyluracil

Synonyms: Borea

Molecular Formula: $C_9H_{13}BrN_2O_2$

Structure:



Chemical Properties

Molecular Weight:	247.12	**Physical State:**	Solid
Vapor Pressure:		**Vapor Density:**	
Boiling Point:	Sublimes	**Melting Point:**	158 to 159°C
Density:		**Solubility:**	815 ppm at 25°C
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 8 x 10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 8

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	3400 mg/kg	rat	oral
LD_{Lo}	3750 mg/kg	mouse	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Bromobenzene

CHEMICAL NAME

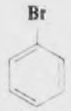
CAS Number: 108-86-1

Chemical Name: Bromobenzene

Synonyms: Phenylbromide

Molecular Formula: C_6H_5Br

Structure:



Chemical Properties

Molecular Weight:	157.02	**Physical State:**	Liquid
Vapor Pressure:	48 mm at 25°C	**Vapor Density:**	5.41
Boiling Point:	156.2°C at 760 mm	**Melting Point:**	-30.5°C
Density:	1.4950 at 20°C/4°C	**Solubility:**	Insoluble (H_2O)
Octanol/Water Partition Coefficient:	2.99		

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–moderate

Bromobenzene

PRODUCTION DATA

Annual U.S. Production:	**Consumption:**
Fraction of Dispersion:	**Fraction of Production Lost:**

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**

Non-lethal Acute Effects:

At high concentrations, may cause paralysis and skin irritation

Chronic Toxicity

U.S. Occupational Standard:

-

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity: **TLV:**

Other Chronic Effects:

Bromonaphthalene

CHEMICAL NAME

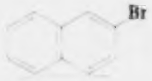
CAS Number: 580-13-2

Chemical Name: 2-Bromonaphthalene

Synonyms:

Molecular Formula: $C_{10}H_7Br$

Structure:



Chemical Properties

Molecular Weight: 207.08

Vapor Pressure: 1 mm at 84.2°C

Boiling Point: 281 to 282°C at 760 mm

Density: 1.605 at 0°C

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 59°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Bromonaphthalene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

1, 3-Butadiene

CHEMICAL NAME

CAS Number: 106-99-0

Chemical Name: 1,3-Butadiene

Synonyms:
Erythrene
Biethylene
Bivinyl
Butadiene
α-β-Butadiene
Divinyl
Pyrrolylene
Vinylethylene

Molecular Formula: C_4H_6

Structure: $CH_2 = CH - CH = CH_2$

Chemical Properties

Molecular Weight: 54.09

Vapor Pressure: 1690 mm at 25°C

Boiling Point: -4.5°C

Density: 0.621 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Gas

Vapor Density: 1.87

Melting Point: -109.91°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–dangerous
Explosion–moderate–forms explosive peroxides with air
Disaster hazard–moderate–toxic fumes

1, 3-Butadiene

PRODUCTION DATA

Annual U.S. Production: 3682.1 x 10^6 lbs. (1974)

Consumption: 4208 x 10^6 lbs.

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 56.9 (1972)

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	250,000 ppm (25 minutes)	human	inhalation

Non-lethal Acute Effects:

Irritant to eyes and mucous membranes
Unconsciousness due to inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA: 1000 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 1000 ppm (skin)

Other Chronic Effects:

Slight irritation of eyes, upper respiratory tract: 8000 ppm (8 hours)

Butane

CHEMICAL NAME

CAS Number: 106-97-8

Chemical Name: Butane

Synonyms:
Methylethylmethane
Butylhydride
Diethyl
n-Butane

Molecular Formula: C_4H_{10}

Structure: $CH_3CH_2CH_2CH_3$

Chemical Properties

Molecular Weight: 58.13

Physical State: Gas

Vapor Pressure: ca. 2

Vapor Density: 2.046

Boiling Point: -0.5°C

Melting Point: -138.35°C

Density: 0.6012 at 0°C/4°

Solubility: 85.98 gm/l of H_2O

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous
Explosion–moderate
Disaster hazard–moderate–toxic fumes

PRODUCTION DATA

Annual U.S. Production: 2331.1 x 10^6 lbs.

Consumption: 2331.1 x 10^6 lbs.

Fraction of Dispersion: 0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 23.3

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	658 mg/m^3	rat	inhalation

Non-lethal Acute Effects:

Drowsiness
Narcotic
Simple asphyxiant

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 500 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

1-Butene

CHEMICAL NAME

CAS Number: 106-98-9

Chemical Name: 1-Butene

Synonyms: 1-Butylene
α-Butylene
Ethylethylene

Molecular Formula: C_4H_8

Structure: $CH_3 - CH_2 - CH = CH_2$

Chemical Properties

Molecular Weight: 56.12

Physical State: Gas

Vapor Pressure: 3480 at 21°C

Vapor Density: 1.93

Boiling Point: –6.3°C at 760 mm

Melting Point: –185.35°C

Density: 0.5951 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous
Explosion–moderate

1-Butene

PRODUCTION DATA

Annual U.S. Production: 2478 x 10^6 lbs. (total butenes)

Consumption: 3960 x 10^6 lbs.

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**

Non-lethal Acute Effects:
Asphyxiant

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

2-Butene (cis and trans)

CHEMICAL NAME

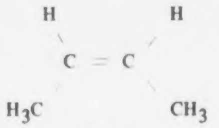
CAS Number: 107-01-7

Chemical Name: 2-Butene

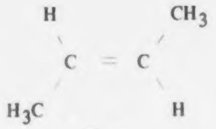
Synonyms: 2-Butene (cis and trans)
Dimethylethylene
Pseudobutylene

Molecular Formula: C_4H_8

Structure:



Cis



Trans

Chemical Properties

Molecular Weight: 56.12

Vapor Pressure: 1410 mm at 21°C (cis)
1592 mm at 21°C (trans)

Boiling Point: 3.7°C at 760 mm (cis)
0.88°C at 760 mm (trans)

Density: 0.6213 at 20°C/4°C (cis)
0.6042 at 20°C/4°C (trans)

Octanol/Water Partition Coefficient:

Physical State: Gas

Vapor Density: 1.9 (cis and trans)

Melting Point: -138.91°C (cis)
-105.55°C (trans)

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous

2-Butene (cis and trans)

PRODUCTION DATA

Annual U.S. Production:	2,478 x 10^6 lbs. (total butenes)	**Consumption:**	3,600 x 10^6 lbs.
Fraction of Dispersion:		**Fraction of Production Lost:**	0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**

Non-lethal Acute Effects:

Simple asphyxiant

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

2-Butoxyethanol

CHEMICAL NAME

CAS Number: 111-76-2

Chemical Name: 2-Butoxyethanol

Synonyms:
- N-butoxyethanol
- 2-Butoxy-l-ethanol
- Ethylene glycol, monobutyl ether
- Monobutyl glycol ether
- Butylglycol
- Butyl oxitol
- o-Butyl ethylene glycol
- 3-Oxa-l-heptanol
- Butyl cellosolve
- Glycol, n-butyl ether

Molecular Formula: $C_6H_{14}O_2$

Structure: $OH - CH_2 - CH_2 - OCH_2 - CH_2 - CH_2 - CH_3$

Chemical Properties

Molecular Weight: 118.18

Vapor Pressure: 0.88 mm at 25°C

Boiling Point: 171.2°C

Density:

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 4.07

Melting Point:

Solubility: 45 gm/l of H_2O

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–moderate

2-Butoxyethanol

PRODUCTION DATA

Annual U.S. Production: 133.3 x 10^6 lbs.

Consumption: 124.3 x 10^6 lbs.

Fraction of Dispersion: 0.97

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 122.6

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1480 mg/kg	rat	oral
	550 mg/kg	rat	intraperitoneal
	340 mg/kg	rat	intravenous
	1230 mg/kg	mouse	oral
	536 mg/kg	mouse	intraperitoneal
	1130 mg/kg	mouse	intravenous
	320 mg/kg	rabbit	oral
	560 mg/kg	rabbit	skin
	280 mg/kg	rabbit	intravenous
	1200 mg/kg	guinea pig	oral
	230 mg/kg	guinea pig	skin
LC_{50}	700 ppm (7 hours)	mouse	inhalation
LC_{Lo}	500 ppm (4 hours)	rat	inhalation
Irritant Effects:			
TD_{Lo}	195 ppm (8 hours)	human	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity: TLV:

Other Chronic Effects:

n-Butyl acetate

CHEMICAL NAME

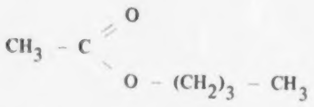
CAS Number: 123-86-4

Chemical Name: Acetic acid, butyl ester

Synonyms: Butyl acetate
Butyl ethanoate
Butyl ester of acetic acid

Molecular Formula: $C_6H_{12}O_2$

Structure:



$CH_3 - C(=O) - O - (CH_2)_3 - CH_3$

Chemical Properties

Molecular Weight: 116.16

Vapor Pressure: 15 mm at 25°C

Boiling Point: 125°C

Density: 0.882 at 20°/20°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point: -77.9

Solubility: 6.29 gm/l of H_2O

Environmental Persistence

BOD: 1.83 for 20 days at 20°C

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate
Explosion–moderate

n-Butyl acetate

PRODUCTION DATA

Annual U.S. Production: 77.2 x 10^6 lbs. (1974)

Consumption: 77.2 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 97.1 (1972)

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1230 mg/kg	mouse	intraperitoneal
LD_{Lo}	1500 mg/kg	rat	intraperitoneal
	3200 mg/kg	rabbit	oral
	4700 mg/kg	guinea pig	oral
Non-lethal Acute Effects:			
Irritant effects–TC_{Lo} Eyes and respiratory tract	200 ppm	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA: 150 ppm

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects: Narcosis

sec-Butyl acetate

CHEMICAL NAME

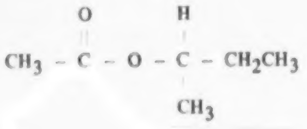
CAS Number: 105-46-4

Chemical Name: Acetic acid, secondary butyl ester

Synonyms: sec-Butyl acetate
2-Butonal acetate

Molecular Formula: $C_6H_{12}O_2$

Structure:



$CH_3 - \overset{\overset{O}{\|}}{C} - O - \underset{\underset{CH_3}{|}}{\overset{\overset{H}{|}}{C}} - CH_2CH_3$

Chemical Properties

Molecular Weight: 116.16

Physical State: Liquid

Vapor Pressure:

Vapor Density: 4.0

Boiling Point: 112.2°C at 760 mm

Melting Point:

Density: 0.8758 at 16°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous
Explosion–moderate

sec-Butyl acetate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 200 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:
Minor allergen and irritant
Moderately toxic if inhaled or ingested

tert-Butyl acetate

CHEMICAL NAME

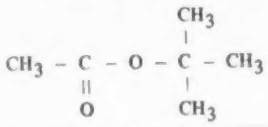
CAS Number: 540-88-5

Chemical Name: Acetic acid, 1,1-dimethylethyl ester

Synonyms: tert-Butyl acetate
Acetic acid, tert-butyl ester

Molecular Formula: $C_6H_{12}O_2$

Structure:



$$CH_3-\underset{\underset{O}{\|}}{C}-O-\overset{\overset{CH_3}{|}}{\underset{\underset{CH_3}{|}}{C}}-CH_3$$

Chemical Properties

Molecular Weight: 116.16

Vapor Pressure:

Boiling Point: 97 to 98°C at 760 mm

Density: 0.8665 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point:

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

tert-Butyl acetate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 200 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Minor allergen and irritant
Moderately toxic if inhaled or ingested

n-Butyl acrylate

CHEMICAL NAME

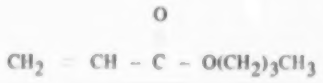
CAS Number: 141-32-2

Chemical Name: Acrylic acid, butyl ester

Synonyms: n-Butyl acrylate
2-Propenoic acid, butyl ester

Molecular Formula: $C_7H_{12}O_2$

Structure:



$CH_2 = CH - \overset{\overset{O}{\|}}{C} - O(CH_2)_3CH_3$

Chemical Properties

Molecular Weight: 128.17

Vapor Pressure: 5.63 mm at 25°C

Boiling Point: 146 to 148°C at 760 mm

Density: 0.8898 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 4.42

Melting Point: –64.6°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–moderate

n-Butyl acrylate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3730 mg/kg	rat	oral
	2000 mg/kg	rabbit	skin
LC_{Lo}	1000 ppm (4 hours)	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

n-Butyl alcohol

CHEMICAL NAME

CAS Number: 71-36-3

Chemical Name: Butyl alcohol

Synonyms:
Butanol
n-Butanol
1-Butanol
Butyl alcohol
Butyl hydroxide
1-Hydroxybutane
Methylolpropane
Propylcarbinol
n-Propylcarbinol

Molecular Formula: $C_3H_{10}O$

Structure: $CH_3 - CH_2 - CH_2 - CH_2 OH$

Chemical Properties

Molecular Weight: 74.12
Vapor Pressure: 7.69 mm at 25°C
Boiling Point: 117 to 118°C at 760 mm
Density: 0.80978 at 20°C/4°C
Octanol/Water Partition Coefficient: 1.00

Physical State: Liquid
Vapor Density: 2.55
Melting Point: -89.0°C
Solubility: Soluble (84.92 gm/l H_2O)

Environmental Persistence

BOD: 2.4 for 20 days at 20°C
Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous
Explosion–moderate
Disaster hazard–moderate–toxic fumes

n-Butyl alcohol

PRODUCTION DATA

Annual U.S. Production: 557.6 x 10^6 lbs.

Consumption: 350 x 10^6 lbs. (1975)

Fraction of Dispersion: 0.23

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 144.6

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	790 mg/kg	rat	oral
LD_{Lo}	970 mg/kg	rat	intraperitoneal
	4250 mg/kg	rabbit	oral

Non-lethal Acute Effects:

Pulmonary effects–TC_{Lo} 25 ppm human inhalation

Irritant–eyes, corneal inflammation, headache, dizziness

Slight irritant–nose and throat

Dermatis–fingernails and finger

Keratitis–reported

Chronic Toxicity

U.S. Occupational Standard: (air) TWA: 100 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:

Eye irritation:	50 ppm
Mild irritation:	25 ppm
Headaches:	50 ppm

sec-Butyl alcohol

CHEMICAL NAME

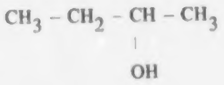
CAS Number: 78-92-2

Chemical Name: sec-Butyl alcohol

Synonyms:
Butan-2-ol
Ethyl methyl carbinol
2-Butyl alcohol
Butylene hydrate
2-Butanol
Methyl ethyl carbinol
s-Butanol
2-Hydroxybutane

Molecular Formula: $C_4H_{10}O$

Structure:



$$CH_3 - CH_2 - \underset{\displaystyle OH}{\underset{|}{CH}} - CH_3$$

Chemical Properties

Molecular Weight: 74.12

Vapor Pressure: 17.5 mm at 25°C

Boiling Point: 99.5

Density: 0.808 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 2.55

Melting Point: -114.7°C

Solubility: 101 gm/l of H_2O

Environmental Persistence

BOD: 2.0 for 50 days at 20°C

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–dangerous

sec-Butyl alcohol

PRODUCTION DATA

Annual U.S. Production: 417 x 10^6 lbs.

Consumption: 417 x 10^6 lbs.

Fraction of Dispersion: 0.05

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 27.1

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	771 mg/kg	mouse	intraperitoneal
LD_{Lo}	6000 mg/kg	rabbit	oral

Chronic Toxicity

U.S. Occupational Standard: (air) TWA: 150 ppm

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV: 150 ppm

Other Chronic Effects:

tert-Butyl alcohol

CHEMICAL NAME

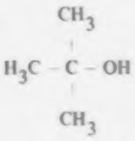
CAS Number: 75-65-0

Chemical Name: tert-Butyl alcohol

Synonyms: 2-Methyl-2 propanol
1,1-Dimethyl ethanol

Molecular Formula: $C_4H_{10}O$

Structure:



$$\begin{array}{ccc} & CH_3 & \\ & | & \\ H_3C - & C & - OH \\ & | & \\ & CH_3 & \end{array}$$

Chemical Properties

Molecular Weight: 74.12

Vapor Pressure: 41.54 at 25°C

Boiling Point: 82.2

Density: 0.7887 at 20°C/4°C

Octanol/Water Partition Coefficient: 0.61

Physical State: Liquid

Vapor Density: 2.55

Melting Point: 25.5°C

Solubility: Infinite (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–dangerous
Explosion–moderate

PRODUCTION DATA

Annual U.S. Production: 1000×10^6 lbs.

Consumption: 1000×10^6 lbs.

Fraction of Dispersion: 0.7

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 715

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3500 mg/kg	rat	oral
	933 mg/kg	mouse	intraperitoneal
LD_{Lo}	4500 mg/kg	rabbit	oral

Chronic Toxicity

U.S. Occupational Standard: (air) TWA: 100 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Human skin contact: slight erythemia and hyperemia

n-Butylaldehyde

CHEMICAL NAME

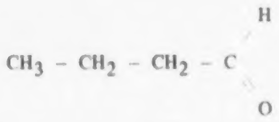
CAS Number: 123-72-8

Chemical Name: Butyraldehyde

Synonyms: n-Butyl aldehyde
Butanal
Butyric aldehyde

Molecular Formula: C_4H_8O

Structure:



$$CH_3 - CH_2 - CH_2 - C\overset{H}{\underset{O}{}}$$

Chemical Properties

Molecular Weight: 72.12

Physical State: Liquid

Vapor Pressure: <10 mm at 25°C

Vapor Density: 2.5

Boiling Point: 75.7°C at 760 mm

Melting Point: -99°C

Density: 0.8170 at 20°C/4°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient: 1.18

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	2490 mg/kg	rat	oral
	2700 mg/kg	mouse	subcutaneous
Non-lethal Acute Effects:			
Irritant			
TC_{Lo}	580 mg/kg	human	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

sec-Butylamine

CHEMICAL NAME

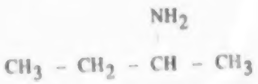
CAS Number: 513-49-5

Chemical Name: (S)2-Butanamine

Synonyms: sec-Butylamine
2-Aminobutane

Molecular Formula: $C_4H_{11}N$

Structure:



$CH_3 - CH_2 - \overset{NH_2}{CH} - CH_3$

Chemical Properties

Molecular Weight: 73.14

Vapor Pressure: 169.8 mm at 25°C

Boiling Point: 63.0°C at 760 mm

Density: 0.724 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point: -104.5°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire –dangerous

sec-Butylamine

PRODUCTION DATA

Annual U.S. Production:	**Consumption:**
Fraction of Dispersion:	**Fraction of Production Lost:**

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	380 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

tert-Butylamine

CHEMICAL NAME

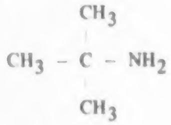
CAS Number: 75-64-9

Chemical Name: t-Butylamine

Synonyms: 2-Aminoisobutane
Trimethylaminomethane

Molecular Formula: $C_4H_{11}N$

Structure:



$$\begin{array}{c} CH_3 \\ | \\ CH_3 - C - NH_2 \\ | \\ CH_3 \end{array}$$

Chemical Properties

Molecular Weight: 73.14

Vapor Pressure: 169.8 mm at 25°C

Boiling Point: 44 to 46°C

Density: 0.700 at 15°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 2.5

Melting Point:

Solubility: Miscible (H_2O)

Environmental Persistence

BOD: 27% of theoretical

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire – moderate

tert-Butylamine

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	180 mg/kg	rat	oral
	900 mg/kg	mouse	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Butylbenzoic acid

CHEMICAL NAME

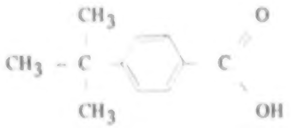
CAS Number: 1320-16-7

Chemical Name: (1,1-Dimethylethyl)benzoic acid

Synonyms:
p-t-BBA
TBBA
p-tert-Butylbenzoic acid
4-tert-Butylbenzoic acid

Molecular Formula: $C_{11}H_{14}O_2$

Structure:



Chemical Properties

Molecular Weight: 178.23

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point: 164.5 to 165.5°C

Density: 1.142 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–slight

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	735 mg/kg	rat	oral

Non-lethal Acute Effects:

Local irritant

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Butylene

CHEMICAL NAME

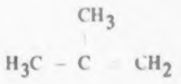
CAS Number: 115-11-7

Chemical Name: 1-Methylpropene

Synonyms: Isobutylene
Isobutene

Molecular Formula: C_4H_8

Structure:



$$H_3C - \overset{\displaystyle CH_3}{\overset{|}{C}} = CH_2$$

Chemical Properties

Molecular Weight: 56.11

Vapor Pressure: 3290 mm at 40.5°C

Boiling Point: -6.9°C

Density: 0.5942 at 20°C/4°C (liquid)

Octanol/Water Partition Coefficient:

Physical State: Gas

Vapor Density: 1.94

Melting Point: -140.35°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire – dangerous
Explosion – dangerous

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Non-lethal Acute Effects:
Simple asphyxiant with narcotic action

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

1, 3-Butylene glycol

CHEMICAL NAME

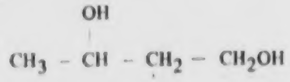
CAS Number: 107-88-0

Chemical Name: 1,3-Butanediol

Synonyms: 1,3-Butylene glycol
β-Butyleneglycol

Molecular Formula: $C_4H_{10}O_2$

Structure:



$$CH_3 - \overset{\displaystyle OH}{\overset{|}{C}H} - CH_2 - CH_2OH$$

Chemical Properties

Molecular Weight: 90.12

Vapor Pressure: 0.06 mm at 20°C

Boiling Point: 207.5°C

Density: 1.006 at 20°C/20°C

Octanol/Water Partition Coefficient: −1.10

Physical State: Liquid

Vapor Density: 3.2

Melting Point:

Solubility: Infinite (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–slight

1, 3-Butylene glycol

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

n-Butyl glycidyl ether

CHEMICAL NAME

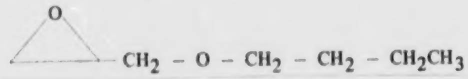
CAS Number: 2426-08-6

Chemical Name: (Butoxymethyl)oxirane

Synonyms: n-Butyl glycidyl ether
BGE
1-Butoxy-2,3-epoxypropane

Molecular Formula: $C_7H_{14}O_2$

Structure:



Chemical Properties

Molecular Weight: 130.21

Vapor Pressure:

Boiling Point: 164°C

Density: 0.91

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point:

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Explosion–dangerous

n-Butyl glycidyl ether

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	2050 mg/kg	rat	oral
	1190 mg/kg	rat	intraperitoneal
	1520 mg/kg	mouse	intraperitoneal
	700 mg/kg	mouse	intraperitoneal
	2520 mg/kg	rabbit	skin
LC_{Lo}	670 ppm	rat	inhalation

Non-lethal Acute Effects:
Irritant to skin

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 50 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 50 ppm or 27 mg/m^3

Other Chronic Effects:

Butylmercaptan

CHEMICAL NAME

CAS Number: 109-71-5

Chemical Name: 1-Butanethiol

Synonyms: n-Butylmercaptan
n-Butyl thioalcohol

Molecular Formula: $C_4H_{10}S$

Structure: $CH_3CH_2CH_2CH_2SH$

Chemical Properties

Molecular Weight:	90.19	**Physical State:**	Liquid
Vapor Pressure:	<10 mm at 25°C	**Vapor Density:**	3.1
Boiling Point:	98.46°C	**Melting Point:**	-115.67°C
Density:	0.8299 at 20°C/4°C	**Solubility:**	Slightly (H_2O)
Octanol/Water Partition Coefficient:	2.28		

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous

Butylmercaptan

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1500 mg/kg	rat	oral
	399 mg/kg	rat	intratracheal
LC_{50}	4020 ppm (4 hours)	rat	inhalation
	2500 ppm (4 hours)	mouse	inhalation
LC_{Lo}	700 ppm (30 minutes)	dog	inhalation
Non-lethal Acute Effects:			
TC_{Lo}	10 mg/m^3 (3 hours)	human	inhalation

Paralysis if concentrated vapor is inhaled

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 10 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

tert-Butylphenol

CHEMICAL NAME

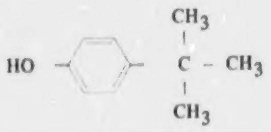
CAS Number: 98-54-4

Chemical Name: p-tert-Butylphenol

Synonyms: Hydroxy-4-tert-butyl benzene

Molecular Formula: $C_{10}H_{14}O$

Structure:



Chemical Properties

Molecular Weight: 150.22

Vapor Pressure: 1 mm at 70°C

Boiling Point: 239.5°C at 760 mm

Density: 0.908 at 80°C/4°C

Octanol/Water Partition Coefficient: 3.31

Physical State: Solid

Vapor Density: 5.1

Melting Point: 101°C

Solubility: Soluble (hot H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

tert-Butylphenol

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	3250 mg/kg	rat	oral
	2520 mg/kg	rabbit	skin

Non-lethal Acute Effects:
Irritant

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

tert-Butyl toluene

CHEMICAL NAME

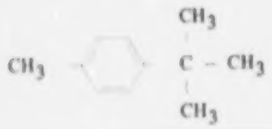
CAS Number: 98-51-1

Chemical Name: p-tert-Butyl toluene

Synonyms: p-Methyl-tert-butylbenzene

Molecular Formula: $C_{11}H_{16}$

Structure:



Chemical Properties

Molecular Weight: 148.25

Physical State: Liquid

Vapor Pressure: <10 mm at 25°C

Vapor Density:

Boiling Point: 193°C at 760 mm

Melting Point: –52°C

Density: 0.8612 at 20°C/4°C

Solubility: Insoluble

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:

Fire–moderate
Disaster hazard–dangerous–toxic fumes

tert-Butyl toluene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1500 mg/kg	rat	oral
	900 mg/kg	mouse	oral
	2000 mg/kg	rabbit	oral
LC_{50}	1500 mg/m^3 (4 hours)	rat	inhalation
	248 ppm (2 hours)	mouse	inhalation
Non-lethal Acute Effects:			
Irritant:			
TC_{Lo}	10 ppm (3 minutes)	human	inhalation
Central nervous system effects:			
TC_{Lo}	20 ppm (5 minutes)	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 10 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 10 ppm

Other Chronic Effects:
Liver and kidneys

n-Butyric acid

CHEMICAL NAME

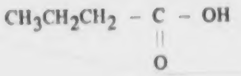
CAS Number: 107-92-6

Chemical Name: Butyric acid

Synonyms: Butanoic acid
Ethyl acetic acid
Propyl formic acid

Molecular Formula: $C_4H_8O_2$

Structure:



$$CH_3CH_2CH_2-\underset{\underset{O}{\|}}{C}-OH$$

Chemical Properties

Molecular Weight: 88.12

Vapor Pressure: 1 mm at 25.5°C

Boiling Point: 163.53°C at 760 mm

Density: 0.9577 at 20°C/4°C

Octanol/Water Partition Coefficient: 0.97

Physical State: Liquid

Vapor Density: 3.04

Melting Point: −4.26°C

Solubility: Infinite (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–moderate

n-Butyric acid

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2400 mg/kg	rat	oral
	3180 mg/kg	mouse	intraperitoneal
	3180 mg/kg	mouse	subcutaneous
	800 mg/kg	mouse	intravenous
LD_{Lo}	500 mg/kg	mouse	oral
	3600 mg/kg	rabbit	oral

Non-lethal Acute Effects:

Irritant to eyes, skin and respiratory tract

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

n-Butyric anhydride

CHEMICAL NAME

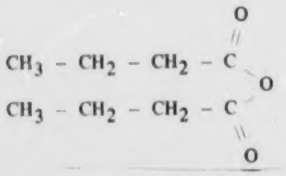
CAS Number: 106-31-0

Chemical Name: Butyric anhydride

Synonyms: n-Butyric anhydride
Butanoic anhydride

Molecular Formula: $C_8H_{14}O_3$

Structure:



$$\begin{array}{l} \qquad\qquad\qquad\qquad\quad O \\ \qquad\qquad\qquad\qquad\quad \| \\ CH_3 - CH_2 - CH_2 - C \\ \qquad\qquad\qquad\qquad\qquad\quad O \\ CH_3 - CH_2 - CH_2 - C \\ \qquad\qquad\qquad\qquad\quad \| \\ \qquad\qquad\qquad\qquad\quad O \end{array}$$

Chemical Properties

Molecular Weight: 158.20

Vapor Pressure: <10 mm at 25°C

Boiling Point: 199.4 to 201.4° at 760 mm

Density: 0.9668 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 5.4

Melting Point: -75°C

Solubility: Decomposes (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire – moderate

n-Butyric anhydride

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Butyronitrile

CHEMICAL NAME

CAS Number: 109-74-0

Chemical Name: Butyronitrile

Synonyms: Butane nitrile
N-propyl cyanide

Molecular Formula: C_4H_7N

Structure: $CH_3 - CH_2CH_2C \equiv N$

Chemical Properties

Molecular Weight: 69.11

Vapor Pressure: 20 mm at 25.7°C

Boiling Point: 118°C at 760 mm

Density: 0.7936 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point: -112°C

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous
Disaster hazard–dangerous–toxic fumes–chlorides

Butyronitrile

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	500 mg/kg	rabbit	skin
LD_{Lo}	50 mg/kg	rat	oral
	100 mg/kg	mouse	oral
	100 mg/kg	guinea pig	skin
LC_{Lo}	400 ppm	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Buxten

CHEMICAL NAME

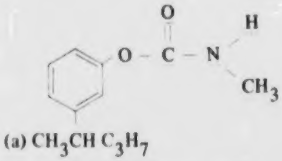
CAS Number: 2282-34-0 (a and b)

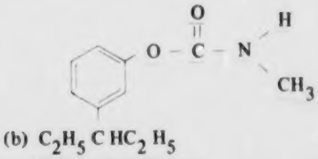
Chemical Name: 3-(1-Methylbutyl)phenol methylcarbamate

Synonyms: Bux
Mixture of (a) m-(1-Methylbutyl)-phenyl methylcarbamate + (b) m-(1-Ethyl propyl)phenyl methylcarbamate

Molecular Formula: $C_{13}H_{19}NO_2$

Structure:


(a) $CH_3CH\ C_3H_7$


(b) $C_2H_5\ C\ HC_2\ H_5$

Chemical Properties

Molecular Weight:	221.33	**Physical State:**	Solid
Vapor Pressure:		**Vapor Density:**	
Boiling Point:		**Melting Point:**	26.4°C
Density:		**Solubility:**	Insoluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Buxten

PRODUCTION DATA

Annual U.S. Production: 6×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 6

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1050 mg/kg	rat	oral
3:1 mixture (a:b)			
LD_{50}	170 mg/kg	rat	oral
	1400 mg/kg	dog	skin
	400 mg/kg	rabbit	skin
4:1 mixture (a:b)			
LD_{50}	87 mg/kg	rat	oral
	242 mg/kg	rat	skin
	1400 mg/kg	dog	skin
	400 mg/kg	rabbit	skin

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Cacodylic acid

CHEMICAL NAME

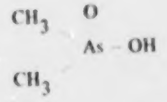
CAS Number: 75-60-5

Chemical Name: Hydroxydimethyl arsine oxide

Synonyms: Dimethyl arsenic acid

Molecular Formula: $C_2H_7AsO_2$

Structure:



$$\begin{array}{ll} CH_3 & O \\ & As-OH \\ CH_3 & \end{array}$$

Chemical Properties

Molecular Weight: 138.01

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 200°C

Solubility: Very soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Disaster hazard–hazardous when water solution is in contact with active metals; i.e., Fe, Al, and Zn.

PRODUCTION DATA

Annual U.S. Production: 2 x 10^6 lbs.

Consumption:

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 2

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1350 mg/kg	rat	oral
	185 mg/kg	mouse	intraperitoneal
LD_{Lo}	500 mg/kg	mouse	unknown
	1000 mg/kg	dog	subcutaneous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Carcinogenic

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Calcium propionate

CHEMICAL NAME

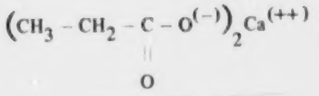
CAS Number: 4075-81-4

Chemical Name: Calcium propionate

Synonyms: Propionic acid, calcium salt

Molecular Formula: $C_6H_{10}O_4 \cdot Ca$

Structure:



$$\left(CH_3 - CH_2 - \underset{\underset{O}{\|}}{C} - O^{(-)}\right)_2 Ca^{(++)}$$

Chemical Properties

Molecular Weight: 186

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point:

Solubility: Soluble (55.8 gm/l H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Calcium propionate

PRODUCTION DATA

Annual U.S. Production: 21.4×10^6 lbs.

Consumption: 21.4×10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 22.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Calcium stearate

CHEMICAL NAME

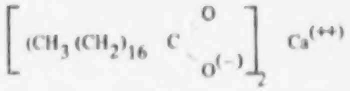
CAS Number. 1592-23-0

Chemical Name: Stearic acid, calcium salt

Synonyms: Calcium salt octadecanoic acid
Calcium stearate

Molecular Formula: $(C_{18}H_{35}O_2)_2 \cdot Ca$

Structure:



$$\left[(CH_3(CH_2)_{16}\, C \overset{O}{\underset{O^{(-)}}{}} \right]_2 Ca^{(++)}$$

Chemical Properties

Molecular Weight: 681.48

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State:

Vapor Density:

Melting Point: 156 to 160°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD: 80% of theoretical for 5 days at 20°C

Atmospheric Reactivity:

Safety Hazard:

Calcium stearate

PRODUCTION DATA

Annual U.S. Production: 37.8×10^6 lbs.

Consumption: 37.8×10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 38.9

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Camphor

CHEMICAL NAME

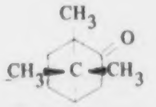
CAS Number: 76-22-2

Chemical Name: Camphor

Synonyms: 2-Camphone

Molecular Formula: $C_{10}H_{16}O$

Structure:



Chemical Properties

Molecular Weight: 152.23

Vapor Pressure: 1 mm at 41.5°C

Boiling Point: 204°C (sublimes)

Density: 0.992 at 25°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density: 5.24

Melting Point: 174 to 179°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–moderate
Explosion–moderate

PRODUCTION DATA

Annual U.S. Production:		**Consumption:**	
Fraction of Dispersion:		**Fraction of Production Lost:**	

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	900 mg/kg	rat	intraperitoneal
LD_{Lo}	2200 mg/kg	mouse	subcutaneous

Non-lethal Acute Effects:

Irritant
Convulsions

Chronic Toxicity

U.S. Occupational Standard: (air) 2 ppm (TWA)

Carcinogenicity: Neoplastic effect

TD_{Lo}	84 mg/kg (1 week)	mouse	skin

Mutagenicity:

Teratogenicity: **TLV:** 5 mg/m^3

Other Chronic Effects:

Caprolactam

CHEMICAL NAME

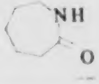
CAS Number: 105-60-2

Chemical Name: Hexahydro-2H-azepin-2-one

Synonyms: 2-Oxohexamethylenimine; 6-Aminohexanoic acid, cyclic lactam; 2-Azacycloheptanone

Molecular Formula: $C_6H_{11}NO$

Structure:



Chemical Properties

Molecular Weight: 113.16

Vapor Pressure: 6 mm at 120°C

Boiling Point: 139°C at 12 mm

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 69 to 71°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Caprolactam

PRODUCTION DATA

Annual U.S. Production: 950 x 10^6 lbs. (1976) capacity

Consumption: 660 x 10^6 lbs.

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	2140 mg/kg	rat	oral
LD_{Lo}	1410 mg/kg	rabbit	skin
	950 mg/kg	guinea pig	subcutaneous
Non-lethal Acute Effects:			
Irritant: TD_{Lo}	7 ppm	human	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Captan

CHEMICAL NAME

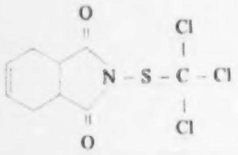
CAS Number: 133-06-2

Chemical Name: N-(Trichloromethyl)thio-4-cyclohexene-1,2-dicarboximide

Synonyms: Cis-N[(trichloromethyl)thio]-4-cyclohexene-1,2-dicarboximide
Tetrahydrophthalimide
Orthocide

Molecular Formula: $C_9H_8Cl_3NO_2S$

Structure:



Chemical Properties

Molecular Weight: 300.62

Vapor Pressure: 0.01μ at 25°C

Boiling Point:

Density: 1.74

Octanol/Water Partition Coefficient: 2.35

Physical State: Solid

Vapor Density:

Melting Point: 175°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 18×10^6 lbs.

Consumption: 18×10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 18.1

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	480 mg/kg	rat	oral
LD_{Lo}	9 mg/kg	mouse	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 5 mg/m^3

Carcinogenicity:

Mutagenicity:

Teratogenicity:				**TLV:**
	3000 mg/kg	pregnant rat	oral	
	38 mg/kg	pregnant rabbit	oral	
	300 mg/kg	pregnant hamster	oral	

Other Chronic Effects:

Carbaryl

CHEMICAL NAME

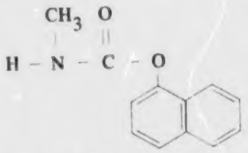
CAS Number: 63-25-2

Chemical Name: Methylcarbamic acid, 1-naphthyl ester

Synonyms: 1-Naphthyl-N-methyl carbamate
Sevin

Molecular Formula: $C_{12}H_{11}NO_2$

Structure:



Chemical Properties

Molecular Weight: 201.24

Vapor Pressure:

Boiling Point:

Density: 1.232 at 20°C/20°C

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 142°C

Solubility:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Carbaryl

PRODUCTION DATA

Annual U.S. Production: 55 x 10^6 lbs.

Consumption: 55 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 55

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	89 mg/kg	rat	oral
	48 mg/kg	rat	intraperitoneal
	500 mg/kg	rat	unknown
	396 mg/kg	mouse	intraperitoneal
	710 mg/kg	rabbit	oral
	280 mg/kg	guinea pig	oral
	197 mg/kg	chicken	oral
	56 mg/kg	wild bird	oral

Non-lethal Acute Effects:

Central nervous system—cholinesterase inhibitor

TD_{Lo}	2800 μg/kg	man	oral

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 5 mg/m^3

Carcinogenicity:

TD_{Lo}	57000 mg/kg (95 wks)	rat	oral
	80 mg/kg	rat	implant

Mutagenicity:

Teratogenicity:			
388 mg/kg	pregnant dog	oral	
300 mg/kg	pregnant guinea pig	oral	
50 mg/kg	pregnant rat	oral	

TVL:

Other Chronic Effects:

Carbofuran

CHEMICAL NAME

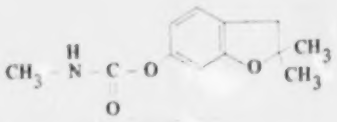
CAS Number: 1563-66-2

Chemical Name: Methyl carbamic acid

Synonyms:
2,3-Dihydro-2,2-dimethyl-7-benzofuranyl
Carbofuran
Methyl carbamate
Furadan

Molecular Formula: $C_{12}H_{15}NO_3$

Structure:



Chemical Properties

Molecular Weight: 2213

Vapor Pressure: 2×10^{-5} mm at 33°C

Boiling Point:

Density: 1.180 at 20°C/20°C

Octanol/Water Partition Coefficient:

Physical State:

Vapor Density:

Melting Point: 150 to 152°C

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Carbofuran

PRODUCTION DATA

Annual U.S. Production: 8×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 8.0

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	11 mg/kg	human	oral
	10 mg/kg	human	skin
	5300 μg/kg	rat	oral
	120 mg/kg	rat	skin
	2 mg/kg	mouse	oral
	19 mg/kg	dog	oral
	885 mg/kg	rabbit	skin
	6 mg/kg	chicken	skin
	415 μg/kg	duck	skin
LC_{50}	85 mg/m^3	rat	inhalation
	52 mg/m^3	dog	inhalation
	32 mg/m^3	guinea pig	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 50 $\mu g/m^3$

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Carbon disulfide

CHEMICAL NAME

CAS Number: 75-15-0

Chemical Name: Carbondisulfide

Synonyms: Carbonbisulfide
Carbondisulphide
Weeviltox

Molecular Formula: CS_2

Structure: $S = C = S$

Chemical Properties

Molecular Weight:	76.13	**Physical State:**	Liquid
Vapor Pressure:		**Vapor Density:**	
Boiling Point:	46.25°C at 760 mm	**Melting Point:**	-111.53°C
Density:	1.2632 at 20°C/4°C	**Solubility:**	Slightly soluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–dangerous
Explosion–dangerous

Carbon disulfide

PRODUCTION DATA

Annual U.S. Production: 767.8 x 10^6 lbs.

Consumption: 752 x 10^6 lbs. (1966)

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{Lo}	300 mg/kg	rabbit	subcutaneous
	400 mg/kg	rat	intraperitoneal
LC_{Lo}	4000 ppm (30 minutes)	human	inhalation
TC_{Lo}	50 mg/m^3	human	inhalation

Chronic Toxicity

U.S. Occupational Standard:

(air) TWA	20 ppm
Ceiling concentration	30 ppm
Peak concentration	100 ppm (30 minutes/8 hours)

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Carbontetrabromide

CHEMICAL NAME

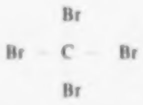
CAS Number: 558-13-4

Chemical Name: Carbon tetrabromide

Synonyms: Tetrabromomethane

Molecular Formula: CBr_4

Structure:



$$\begin{array}{ccc} & Br & \\ Br - & C & - Br \\ & Br & \end{array}$$

Chemical Properties

Molecular Weight: 331.67

Vapor Pressure: 44 mm at 96.3°C

Boiling Point: 189.5°C

Density: 3.42

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 90.1°C

Solubility: Soluble (H_2O) (785 mg/l at 20°C)

Environmental Persistence

BOD: No oxygen consumption in standard testing

Atmospheric Reactivity: Reacts with oxidizing materials.

Safety Hazard: Disaster hazard–dangerous–toxic fumes

Carbontetrabromide

PRODUCTION DATA

Annual U.S. Production: 1000 x 10^6 lbs. (1970)

Consumption: 1000 x 10^6 lbs.

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 60

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	298 mg/kg	mouse	subcutaneous
LD_{Lo}	1000 mg/kg	rat	oral

Non-lethal Acute Effects:
Narcotic in high concentrations

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 100 ppb

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Carbon tetrachloride

CHEMICAL NAME

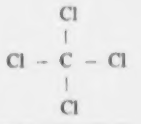
CAS Number: 56-23-5

Chemical Name: Carbon tetrachloride

Synonyms: Tetrachloromethane
Perchloromethane
Methane tetrachloride

Molecular Formula: CCl_4

Structure:



$$\begin{array}{c} Cl \\ | \\ Cl - C - Cl \\ | \\ Cl \end{array}$$

Chemical Properties

Molecular Weight: 153.82

Vapor Pressure: 115.2 mm at 25°C

Boiling Point: 76.54°C at 760 mm

Density: 1.5940 at 20°C/4°C

Octanol/Water Partition Coefficient: 2.64

Physical State: Liquid

Vapor Density: 5.32

Melting Point: -22.99°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD: No O_2 consumption in standard BOD test

Atmospheric Reactivity:
Photodegradation: $t_{1/2}$ = 10 to 33 weeks

Safety Hazard:

Carbon tetrachloride

PRODUCTION DATA

Annual U.S. Production: 1,047 x 10^6 lbs. (1973)

Consumption: 989.3 x 10^6 lbs.

Fraction of Dispersion: 0.05

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 65

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1770 mg/kg	rat	oral
	4620 mg/kg	mouse	intraperitoneal
	6380 mg/kg	rabbit	oral
LD_{Lo}	3200 mg/kg	mouse	subcutaneous
	1000 mg/kg	dog	oral
	125 mg/kg	dog	intravenous
	4785 mg/kg	cat	subcutaneous
	3000 mg/kg	rabbit	subcutaneous
LC_{50}	9526 ppm (8 hours)	mouse	inhalation
LC_{Lo}	38,110 ppm (2 hours)	cat	inhalation
	550 ppm	rabbit	inhalation
	20,000 ppm (2 hours)	guinea pig	inhalation
	1,000 ppm	human	inhalation
	4,000 ppm (4 hours)	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard:

(air) TWA: 10 ppm
Ceiling level: 25 ppm
Peak concentration: 200 ppm/5 minutes/4 hours

Carcinogenicity:

Neoplastic effects:			
TD_{Lo}	133 gm/kg (25 weeks, intermittent)	rat	subcutaneous
Carcinogenicity:			
TD_{Lo}	4800 mg/kg (88 days, intermittent)	mouse	oral

Mutagenicity:
Positive

Teratogenicity:

TLV. 10 ppm
Odor perception: 77 ppm

Other Chronic Effects:

Castor oil

CHEMICAL NAME

CAS Number: 8001-79-4

Chemical Name: Castor oil

Synonyms: Ricinus oil
Ricinolein
Glycerides of ricinoleic and isoricinoleic acids

Molecular Formula: (not given in CAS Registry Number Handbook, since the composition varies)

Structure:

$[CH_3(CH_2)_5CH=CHCH=CH(CH_2)_7COO]_3C_3H_5$

Chemical Properties

Molecular Weight: (Varies)

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 313°C (decomposes)

Melting Point: -10°C

Density: 0.96 at 25° C/25°C

Solubility: <5.0 gm/l H_2O (Insoluble)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–slight

PRODUCTION DATA

Annual U.S. Production: 100×10^6 lbs.

Consumption: 198×10^6 lbs.

Fraction of Dispersion: 0.64

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 129.7 (1972)

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
(Low toxicity)			

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Cellulose acetate

CHEMICAL NAME

CAS Number: 9004-35-7

Chemical Name: Cellulose acetate

Synonyms:
CA
Acetate ester of cellulose
Acetic acid, cellulose ester
Acetyl cellulose

Molecular Formula: (Exact composition unknown or undetermined)

Structure: (Cellulose ester in which the cellulose is not completely esterified by the acetic acid.)

Chemical Properties

Molecular Weight: (undetermined)

Vapor Pressure: Negligible

Boiling Point:

Density: 1.27 to 1.34

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 260°C (decomposes)

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire - moderate

PRODUCTION DATA

Annual U.S. Production: 807.1 x 10^6 lbs.

Consumption: 820.4 x 10^6 lbs.

Fraction of Dispersion: 0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 24.6

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
(Nontoxic)			

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Chloranil

CHEMICAL NAME

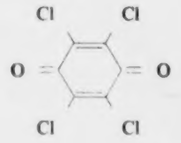
CAS Number: 118-75-2

Chemical Name: 2,3,5,6-Tetrachloro-p-benzoquinone

Synonyms: Tetrachloroquinone
Dow seed disinfectant No. 5

Molecular Formula: $C_6Cl_4O_2$

Structure:



Chemical Properties

Molecular Weight: 245.9	**Physical State:** Solid
Vapor Pressure: 1 mm at 70.7°C	**Vapor Density:**
Boiling Point: Sublimes	**Melting Point:** 290°C (sealed tube)
Density:	**Solubility:** Insoluble (H_2O)
Octanol/Water Partition Coefficient:	

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Disaster hazard–dangerous toxic fumes–chloride

Chloranil

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	4000 mg/kg	rat	oral
	500 mg/kg	rat	intraperitoneal
LD_{Lo}	4 mg/kg	mouse	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Chlordane

CHEMICAL NAME

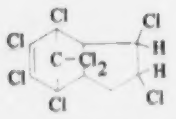
CAS Number: 57-74-9

Chemical Name: 1,2,4,5,6,7,8,8-Octachloro-3a,4,7,7a-tetrahydro-4,7-methanoindane

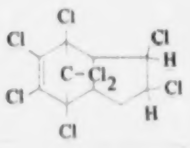
Synonyms: Chlordane
Octaklor
Gama-chlordan

Molecular Formula: $C_{10}H_8Cl_8$

Structure:



α Trans



β Cis

Chemical Properties

Molecular Weight: 409.76

Vapor Pressure: 1×10^{-5} mm at 25°C

Boiling Point: 175°C

Density: 1.57 to 1.63 at 15.5°C/15.5°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point:

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 25 x 10^6 lbs.

Consumption: 25 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 25.3

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	283 mg/kg	rat	oral
	700 mg/kg	rat	skin
	200 mg/kg	rat	intraperitoneal
	430 mg/kg	mouse	oral
	100 mg/kg	rabbit	oral
	220 mg/kg	chicken	oral
LD_{Lo}	40 mg/kg	human	oral

Non-lethal Acute Effects:

CNS stimulant

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 500 $\mu g/m^3$

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 0.5 mg/m^3

Other Chronic Effects: Liver damage
Kidney damage

Chloroacetaldehyde

CHEMICAL NAME

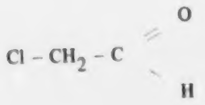
CAS Number: 107-20-0

Chemical Name: Chloroacetaldehyde

Synonyms: Chloroaldehyde
2-Chloro-1-ethanal

Molecular Formula: C_2H_3ClO

Structure:



$$\mathrm{Cl-CH_2-C}\begin{matrix} ^{\diagup\!\!\diagup}\mathrm{O} \\ _{\diagdown}\mathrm{H}\end{matrix}$$

Chemical Properties

Molecular Weight: 78.5

Vapor Pressure: 100 mm at 45°C

Boiling Point: 85 to 85.5°C at 748 mm

Density: 1.19 at 25°C/25°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point:

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–moderate

Chloroacetaldehyde

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	23 mg/kg	rat	oral
	2 mg/kg	rat	intraperitoneal
	21 mg/kg	mouse	oral
	2 mg/kg	mouse	intraperitoneal
	67 mg/kg	rabbit	skin
	1390 mg/kg	rabbit	intraperitoneal
	636 mg/kg	guinea pig	intraperitoneal

Non-lethal Acute Effects:

Irritant to eyes, skin respiratory organs and mucous membranes

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 1 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Chloroacetic acid

CHEMICAL NAME

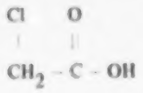
CAS Number: 79-11-8

Chemical Name: Chloroacetic acid

Synonyms: Monochloroacetic acid

Molecular Formula: $C_2H_3Cl\,O_2$

Structure:



$$\overset{\displaystyle Cl}{\overset{|}{CH_2}} - \overset{\displaystyle O}{\overset{\|}{C}} - OH$$

Chemical Properties

Molecular Weight: 94.50

Vapor Pressure: 1 mm at 23°C

Boiling Point: 187.85°C

Density: 1.4043 at 40°C/4°C

Octanol/Water Partition Coefficient: 1.83

Physical State: Solid

Vapor Density: 3.26

Melting Point: 63.0°C

Solubility: Very soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Disaster hazard–dangerous–toxic fumes–phosgene and chlorides

Chloroacetic acid

PRODUCTION DATA

Annual U.S. Production: 84 x 10^6 lbs. (capacity)

Consumption: 96 x 10^6 lbs. (1975)

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	76 mg/kg	rat	oral
	5 mg/kg	rat	subcutaneous
LD_{Lo}	500 mg/kg	mouse	intraperitoneal

Non-lethal Acute Effects:
Irritant

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Chloroacetophenone

CHEMICAL NAME

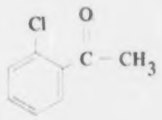
CAS Number: 532-27-4

Chemical Name: 2-Chloroacetophenone

Synonyms: o-Chlorophenyl methyl ketone

Molecular Formula: C_8H_7ClO

Structure:



Chemical Properties

Molecular Weight: 154.60

Vapor Pressure: 1 mm at 48°C

Boiling Point: 227 to 228°C at 738 mm

Density: 1.2016 at 17°C/4°C

Octanol/Water Partition Coefficient: 2.08

Physical State: Solid or liquid

Vapor Density:

Melting Point:

Solubility:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Chloroacetophenone

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
Non-lethal Acute Effects:	Irritant		
TC_{Lo}	93 mg/m^3 (3 minutes)	human	inhalation
	20 mg/m^3 (3 minutes)	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) Ceiling concentration 0.05 ppm

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

m-Chloroaniline

CHEMICAL NAME

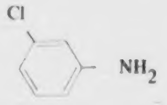
CAS Number: 108-42-9

Chemical Name: m-Chloroaniline

Synonyms: 3-Chloroaniline

Molecular Formula: C_6H_6ClN

Structure:



Chemical Properties

Molecular Weight: 127.52

Vapor Pressure: 1 mm at 63.5°C

Boiling Point: 230.5°C

Density: 1.223 at 15°C/15°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point: -10.6°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

m-Chloroaniline

PRODUCTION DATA

Annual U.S. Production:	**Consumption:**
Fraction of Dispersion:	**Fraction of Production Lost:**

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	880 mg/kg	rat	oral
LD_{Lo}	310 mg/kg	cat	subcutaneous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity: **TLV:**

Other Chronic Effects:

o-Chloroaniline

CHEMICAL NAME

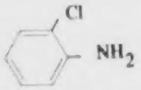
CAS Number: 95-51-2

Chemical Name: o-Chloroaniline

Synonyms: 2-Chloroaniline

Molecular Formula: C_6H_6ClN

Structure:



Chemical Properties

Molecular Weight: 127.52

Vapor Pressure: 1 mm at 63.5°C

Boiling Point: 208.84

Density:

Octanol/Water Partition Coefficient: 1.2125 at 20°C/4°C

Physical State: Liquid

Vapor Density:

Melting Point: 2.3°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

o-Chloroaniline

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	256 mg/kg	mouse	oral
LD_{Lo}	310 mg/kg	cat	subcutaneous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

p-Chloroaniline

CHEMICAL NAME

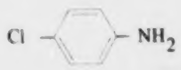
CAS Number: 106-47-8

Chemical Name: p-Chloroaniline

Synonyms: 4-Chloroaniline

Molecular Formula: C_6H_6ClN

Structure:



Chemical Properties

Molecular Weight: 127.52

Vapor Pressure: 1 mm at 63.5°C

Boiling Point: 232°C at 760mm

Density: 1.429 at 19°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 69.5°C

Solubility: Soluble (hot H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

p-Chloroaniline

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	300 mg/kg	rat	oral
	420 mg/kg	rat	intraperitoneal
	100 mg/kg	mouse	oral
	100 mg/kg	wild bird	oral
LD_{Lo}	125 mg/kg	cat	subcutaneous
	36 mg/kg	rabbit	skin

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

o-Chlorobenzaldehyde

CHEMICAL NAME

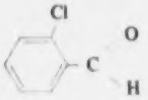
CAS Number: 89-98-5

Chemical Name: o-Chlorobenzaldehyde

Synonyms: 2-Chlorobenzaldehyde

Molecular Formula: C_7H_5ClO

Structure:



Chemical Properties

Molecular Weight: 140.57	**Physical State:** Liquid
Vapor Pressure: 10 mm at 25°C	**Vapor Density:**
Boiling Point: 211.9°C at 760 mm	**Melting Point:** 12.39°C
Density: 1.2483 at 20°C/4°C	**Solubility:** Slightly soluble (H_2O)
Octanol/Water Partition Coefficient:	

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

o-Chlorobenzaldehyde

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	10 mg/kg	mouse	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

p-Chlorobenzaldehyde

CHEMICAL NAME

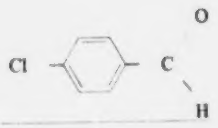
CAS Number: 104-88-1

Chemical Name: p-Chlorobenzaldehyde

Synonyms:

Molecular Formula: C_7H_5ClO

Structure:



Chemical Properties

Molecular Weight: 140.57	**Physical State:** Solid
Vapor Pressure:	**Vapor Density:**
Boiling Point: 213 to 214°C at 760 mm	**Melting Point:** 47.5°C
Density: 1.196 at 61°C/4°C	**Solubility:** Soluble (H_2O)
Octanol/Water Partition Coefficient:	

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

p-Chlorobenzaldehyde

PRODUCTION DATA

Annual U.S. Production:	**Consumption:**
Fraction of Dispersion:	**Fraction of Production Lost:**

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Chlorobenzene

CHEMICAL NAME

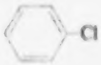
CAS Number: 108-90-7

Chemical Name: Chlorobenzene

Synonyms: Phenyl chloride
Monochlorobenzene
Chlorobenzol

Molecular Formula: C_6H_5Cl

Structure:



Chemical Properties

Molecular Weight: 112.56	**Physical State:** Liquid
Vapor Pressure: 12.14 mm at 25°C	**Vapor Density:** 3.88
Boiling Point: 131.7°C at 760 mm	**Melting Point:** –45.6°C
Density: 1.1058 at 20°C/4°C	**Solubility:** Insoluble (H_2O)
Octanol/Water Partition Coefficient: 2.84	

Environmental Persistence

BOD: 1% of theoretical

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–dangerous
Explosion–moderate

Chlorobenzene

PRODUCTION DATA

Annual U.S. Production: 690 x 10^6 lbs. (1976 capacity)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2910 mg/kg	rat	oral
	2830 mg/kg	rabbit	oral
LD_{Lo}	4000 mg/kg	rat	subcutaneous

Non-lethal Acute Effects:

Strong narcotic

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 75 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 75 ppm

Other Chronic Effects: Kidney damage
Liver damage

Chlorobenzilate

CHEMICAL NAME

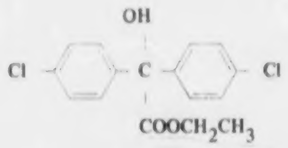
CAS Number: 510-15-6

Chemical Name: 4,4′-Dichlorobenzilic acid, ethyl ester

Synonyms: Acaradben
Benzilic acid, 4,4′-dichloroethyl ester
Chlorobenzilate

Molecular Formula: $C_{16}H_{14}Cl_2O_3$

Structure:



Chemical Properties

Molecular Weight: 325.20

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 148°C at 0.04 mm

Melting Point:

Density:

Solubility:

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Chlorobenzilate

PRODUCTION DATA

Annual U.S. Production: 2×10^6 lbs

Consumption:

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 2.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	700 mg/kg	rat	oral
	724 mg/kg	mouse	oral
LC_{50}	500 ppm	mammal	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: TD_{Lo} 71 mg/kg (82 weeks) mouse oral

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Chlorobenzoic acid

CHEMICAL NAME

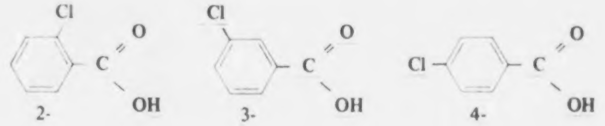
CAS Number:
2-: 118-91-2
3-: 535-80-8
4-: 74-11-3

Chemical Name: Chlorobenzoic acid (2-, 3- and 4-)

Synonyms: Chlorobenzoic acid (o-, m-, and p-)

Molecular Formula: $C_7H_5ClO_2$

Structure:



Chemical Properties

Molecular Weight: 156.57

Vapor Pressure:

Boiling Point: (2-) and (3-) sublime

Density: (2-) 1.544 gm/ml (20°C)
(3-) 1.496 gm/mg (25°C/4°C)

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: (2-) 142°C (3-) 158°C
(4-) 243°C

Solubility: (2-) Slightly soluble in hot water
(3-) Very soluble in hot water
(4-) Slightly soluble in hot water

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Chlorobenzoic acid

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

o-Chlorobenzoyl chloride

CHEMICAL NAME

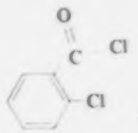
CAS Number: 609-65-4

Chemical Name: o-Chlorobenzoyl chloride

Synonyms: 2-Chlorobenzoic acid chloride

Molecular Formula: $C_7H_4Cl_2O$

Structure:



Chemical Properties

Molecular Weight: 175.02

Vapor Pressure:

Boiling Point: 238°C at 760 mm

Density: 1.270 to 1.280 at 25°C/15°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 5.55

Melting Point: -4 to -6°C

Solubility: Decomposes (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

o-Chlorobenzoyl chloride

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

o-Chlorobenzylidene malononitrile

CHEMICAL NAME

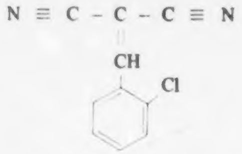
CAS Number: 18270-61-6

Chemical Name: o-Chlorobenzylidene malonitrile

Synonyms: OCBM

Molecular Formula: $C_{10}H_5ClN_2$

Structure:



Chemical Properties

Molecular Weight: 188.62	**Physical State:** Solid
Vapor Pressure:	**Vapor Density:**
Boiling Point: 313°C	**Melting Point:**
Density:	**Solubility:**
Octanol/Water Partition Coefficient:	

Environmental Persistence

BOD:

Atmospheric Reactivity

Safety Hazard:

o-Chlorobenzylidene malononitrile

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	178 mg/kg	rat	oral
	48 mg/kg	rat	intraperitoneal
	35 mg/kg	rat	intravenous
LD_{Lo}	282 mg/kg	mouse	oral
	50 mg/kg	mouse	intraperitoneal
	8 mg/kg	rabbit	intravenous

Non-lethal Acute Effects:

Central nervous system–TC_{Lo} 1500 mg/m^3 (90 minutes) human inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Chlorodifluoroethane

CHEMICAL NAME

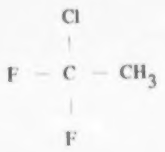
CAS Number: 75-68-3

Chemical Name: Chlorodifluoroethane

Synonyms: 1 Chloro-1, 1-difluoroethane

Molecular Formula: $C_2H_3ClF_2$

Structure:



$$\begin{array}{ccccc} & & Cl & & \\ & & | & & \\ F & - & C & - & CH_3 \\ & & | & & \\ & & F & & \end{array}$$

Chemical Properties

Molecular Weight: 100.50

Vapor Pressure:

Boiling Point: -9.2°C

Density:

Octanol/Water Partition Coefficient:

Physical State: Gas

Vapor Density:

Melting Point: -130.8°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Chlorodifluoroethane

PRODUCTION DATA

Annual U.S. Production: 0.2 x 10^6 lbs. (1972)

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Asphyxiant at high concentrations

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Chlorodifluoromethane

CHEMICAL NAME

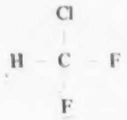
CAS Number: 75-45-6

Chemical Name: Chlorodifluoromethane

Synonyms: Freon-22
Fluorocarbon-22

Molecular Formula: $CHClF_2$

Structure:



$$\begin{array}{ccccc} & & Cl & & \\ & & | & & \\ H & - & C & - & F \\ & & | & & \\ & & F & & \end{array}$$

Chemical Properties

Molecular Weight: 86.5

Vapor Pressure: 2210.6 mm at 25°C

Boiling Point: -40.8°C

Density: 3.87 that of air at 0°C

Octanol/Water Partition Coefficient:

Physical State: Gas

Vapor Density:

Melting Point: -160°C

Solubility: Partly soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Chlorodifluoromethane

PRODUCTION DATA

Annual U.S. Production: 80 x 10^6 lbs. (1972)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Asphyxiant at high concentrations

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

2-Chloro-4-ethylamino-6-isopropylamino-s-triazine

CHEMICAL NAME

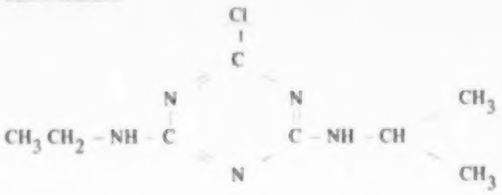
CAS Number: 1912-24-9

Chemical Name: 2-Chloro-4-(ethylamino)-6-isopropylamino-s-triazine

Synonyms: Atrazine

Molecular Formula: $C_8H_{14}Cl\,N_5$

Structure:



Chemical Properties

Molecular Weight: 215.72

Physical State: Solid

Vapor Pressure: 3.0×10^{-7} Torrs at 20°C

Vapor Density:

Boiling Point:

Melting Point: 175°C

Density:

Solubility: Slightly (hot H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

2-Chloro-4-ethylamino-6-isopropylamino-s-triazine

PRODUCTION DATA

Annual U.S. Production: 110 x 10^6 lbs.

Consumption: 110 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 111.1

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1750 mg/kg	rat	oral
	1750 mg/kg	mouse	oral
	3080 mg/kg	rat	unknown

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Chloroform

CHEMICAL NAME

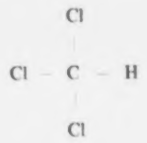
CAS Number: 67-66-3

Chemical Name: Chloroform

Synonyms: Trichloromethane
Methenyl chloride

Molecular Formula: $CHCl_3$

Structure:



$$\begin{array}{ccccc} & & \mathrm{Cl} & & \\ & & | & & \\ \mathrm{Cl} & - & \mathrm{C} & - & \mathrm{H} \\ & & | & & \\ & & \mathrm{Cl} & & \end{array}$$

Chemical Properties

Molecular Weight: 119.39

Vapor Pressure: 200 mm at 25.9°C

Boiling Point: 61.26°C

Density: 1.49845 at 15°C

Octanol/Water Partition Coefficient: 1.17

Physical State: Liquid

Vapor Density: 4.12

Melting Point: -63.5°C

Solubility: Soluble (H_2O) (8.0 gm/l)

Environmental Persistence

BOD: 4% of theoretical for 5 days at 20°C
Total theoretical oxygen demand gm/gm=0.19

Atmospheric Reactivity: Activity toward OH: $t_{1/2} = >1$ yr.

Safety Hazard: Fire–Slight
Disaster hazard–dangerous–toxic fumes–phosgene

Chloroform

PRODUCTION DATA

Annual U.S. Production: 234.7 x 10^6 lbs.

Consumption: 234.7

Fraction of Dispersion: 0.70

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 167.8

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	800 mg/kg		
	704 mg/kg		
LD_{Lo}	2500 mg/kg	mouse	oral
	1000 mg/kg	dog	oral
	75 mg/kg	dog	intravenous
	800 mg/kg	rabbit	subcutaneous
LC_{50}	28 ppm	mouse	inhalation
	100 ppm	dog	inhalation
	59 ppm	rabbit	inhalation
LC_{Lo}	8000 ppm (4 hours)	rat	inhalation
	20000 ppm (2 hours)	guinea pig	inhalation

Non-lethal Acute Effects:

Systemic effects (Liver or kidney)	10 ppm (1 year)	human	inhalation
Motor reflexes–rabbit			
Kidney, liver and vascular lesions			

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 50 ppm, but NIOSH has recommended TWA 10 ppm

Carcinogenicity: TD_{Lo} 18 gm/kg (120 days) mouse oral

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:
Irritation of eyes and mucous membranes
CNS paralysis after prolonged exposure
Placental lesions
Alteration in neuroendocrine system

Chloronaphthalene

CHEMICAL NAME

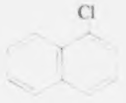
CAS Number: 90-13-1

Chemical Name: 1-Chloronaphthalene

Synonyms: α-Chloronaphthalene
Chloronaphthalene

Molecular Formula: $C_{10}H_7Cl$

Structure:



Chemical Properties

Molecular Weight: 162.61	**Physical State:** Liquid
Vapor Pressure: 1 mm at 80.6°C	**Vapor Density:**
Boiling Point: 259°C at 753mm	**Melting Point:** -2.3°C
Density: 1.1938 at 20°C/4°C	**Solubility:** Insoluble (H_2O)
Octanol/Water Partition Coefficient:	

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–slight

Chloronaphthalene

PRODUCTION DATA

Annual U.S. Production: 5 x 10^6 lbs. (1972)

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1540 mg/kg	rat	oral
	1091 mg/kg	mouse	oral

Non-lethal Acute Effects:

Conjunctivitis
Jaundice
Vomiting
Highly toxic by ingestion, inhalation, and skin absorption
Strong irritant

Chronic Toxicity

U.S. Occupational Standard:
(Tolerance: 2 mg/m^3)

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

m-Chloronitrobenzene

CHEMICAL NAME

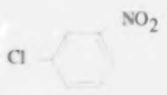
CAS Number: 88-73-3

Chemical Name: 1-Chloro-3-nitrobenzene

Synonyms: m-Chloronitrobenzene

Molecular Formula: $C_6H_4ClNO_2$

Structure:



Chemical Properties

Molecular Weight: 157.6

Physical State: Solid

Vapor Pressure: <10 mm at 25°C

Vapor Density:

Boiling Point: 236°C

Melting Point: 44°C

Density: 1.534 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient: 2.41

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–slight
Disaster hazard–dangerous–toxic fumes–nitrate and phosgene

m-Chloronitrobenzene

PRODUCTION DATA

Annual U.S. Production: 142 x 10^6 lbs. (1967)

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	288 mg/kg	rat	oral
	135 mg/kg	mouse	oral

Non-lethal Acute Effects:

Eye TC_{Lo}	12 mg/m^3	human	inhalation

Intoxication
Methemoglobin, cyanosis and blood changes
Poisoning by pulmonary route
Irritation of nose and throat

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV: 1 ppm

Other Chronic Effects:

o-Chloronitrobenzene

CHEMICAL NAME

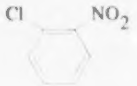
CAS Number: 88-73-3

Chemical Name: 1-Chloro-2-nitrobenzene

Synonyms: 1-Chloro-2-nitrobenzene

Molecular Formula: $C_6H_4ClNO_2$

Structure:



Chemical Properties

Molecular Weight: 157.6

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 245 to 246°C at 760 mm

Melting Point: 33.5 to 35.0°C

Density: 1.305

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–slight
Disaster hazard–dangerous–toxic fumes–nitrate and phosgene

o-Chloronitrobenzene

PRODUCTION DATA

Annual U.S. Production: 142 x 10^6 lbs. (1967)

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	288 mg/kg	rat	oral
	135 mg/kg	mouse	oral

Non-lethal Acute Effects:

Anemia
Irritation of eyes, nose, and throat

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 1 ppm

Other Chronic Effects:

p-Chloronitrobenzene

CHEMICAL NAME

CAS Number: 100-00-5

Chemical Name: 1-Chloro-4-nitrobenzene

Synonyms: p-Chloronitrobenzene
p-Nitrochlorobenzene

Molecular Formula: $C_6H_4ClNO_2$

Structure:

Chemical Properties

Molecular Weight: 157.6	**Physical State:** Solid
Vapor Pressure: 10 mm at 25°C	**Vapor Density:** 5.43
Boiling Point: 242°C	**Melting Point:** 83°C
Density: 1.520 at 22°C/4°C	**Solubility:** insoluble (H_2O)
Octanol/Water Partition Coefficient: 2.41	

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire—slight
Disaster hazard—dangerous—toxic fumes—nitrate and chlorides

p-Chloronitrobenzene

PRODUCTION DATA

Annual U.S. Production: 142 x 10^6 lbs. (1967)

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1414 mg/kg	mouse	oral
	420 mg/kg	mammal	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 1 mg/m^3

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

1-Chloro-1-nitropropane

CHEMICAL NAME

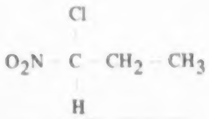
CAS Number: 600-25-9

Chemical Name: 1-Chloro-1-nitropropane

Synonyms:

Molecular Formula: $C_3H_6ClNO_2$

Structure:



$$O_2N-\overset{\displaystyle Cl}{\underset{\displaystyle H}{C}}-CH_2-CH_3$$

Chemical Properties

Molecular Weight: 123.5

Vapor Pressure:

Boiling Point: 139.5°C

Density: 1.209 at 20°C/20°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 4.26

Melting Point:

Solubility: Slightly soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–moderate
Explosion–dangerous
Disaster hazard–toxic fumes

1-Chloro-1-nitropropane

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	510 mg/kg	mouse	oral
LD_{Lo}	165 mg/kg	mouse	subcutaneous
	50 mg/kg	rabbit	oral

Non-lethal Acute Effects:

Irritant
Severe pulmonary edema after inhalation or ingestion

Chronic Toxicity

U.S. Occupational Standard: (air) 20 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

m-Chlorophenol

CHEMICAL NAME

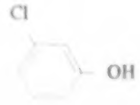
CAS Number: 108-43-0

Chemical Name: m-Chlorophenol

Synonyms: 3-Chlorophenol

Molecular Formula: C_6H_5ClO

Structure:



Chemical Properties

Molecular Weight: 128.6

Vapor Pressure: 1 mm at 44.2°C

Boiling Point: 214°C

Density: 1.268 at 25°C

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 33°C

Solubility: Slightly soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Disaster hazard – toxic fumes

PRODUCTION DATA

Annual U.S. Production:	**Consumption:**
Fraction of Dispersion:	**Fraction of Production Lost:**
Release Rate (million lbs/yr):	

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	570 mg/kg	rat	oral
	355 mg/kg	rat	intraperitoneal
	1390 mg/kg	rat	subcutaneous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:	**TLV:**

Other Chronic Effects:
Irritant

o-Chlorophenol

CHEMICAL NAME

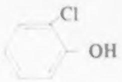
CAS Number: 95-57-8

Chemical Name: o-Chlorophenol

Synonyms: 2-Chlorophenol

Molecular Formula: C_6H_5ClO

Structure:



Chemical Properties

Molecular Weight:	128.6	**Physical State:**	Liquid
Vapor Pressure:	2.97 at 25°C	**Vapor Density:**	
Boiling Point:	174.5°C	**Melting Point:**	7°C
Density:	1.256 at 25°C/25°C	**Solubility:**	Slightly (H_2O)
Octanol/Water Partition Coefficient:	2.19		

Environmental Persistence

BOD: 100% of theoretical after 36 days

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

o-Chlorophenol

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	670 mg/kg	rat	oral
	230 mg/kg	rat	intraperitoneal
	950 mg/kg	rat	subcutaneous
	670 mg/kg	mouse	oral
	440 mg/kg	mammal	oral
LD_{Lo}	950 mg/kg	rabbit	subcutaneous
	800 mg/kg	guinea pig	subcutaneous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Neoplastic effect TD_{Lo} 38 gm/kg (12 weeks) mouse skin

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

p-Chlorophenol

CHEMICAL NAME

CAS Number: 106-48-9

Chemical Name: p-Chlorophenol

Synonyms: 4-Chlorophenol

Molecular Formula: C_6H_5ClO

Structure:

Chemical Properties

Molecular Weight: 128.56

Vapor Pressure: 1 mm at 49.8°C

Boiling Point: 220°C

Density: 1.246 at 60°C/25°C

Octanol/Water Partition Coefficient: 2.44

Physical State: Solid

Vapor Density:

Melting Point: 42 to 43°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD: 100% of theoretical after 36 days

Atmospheric Reactivity:

Safety Hazard: Fire moderate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	500 mg/kg	rat	oral
	281 mg/kg	rat	intraperitoneal
	1030 mg/kg	rat	subcutaneous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Chloroprene

CHEMICAL NAME

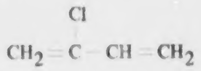
CAS Number: 126-99-8

Chemical Name: 2-Chloro-1,3-butadiene

Synonyms: 2-Chlorobutadiene-1,3
β-Chloroprene
Chloroprene

Molecular Formula: C_4H_5Cl

Structure:



$CH_2=\overset{Cl}{\overset{|}{C}}-CH=CH_2$

Chemical Properties

Molecular Weight: 88.54

Vapor Pressure: 215.4 mm at 25°C

Boiling Point: 59.4°C

Density: 0.9583 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point:

Solubility: Slightly <10.0 gm/l (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:
Activity toward RO_2 $t_{1/2} = 2.2$ yrs.
O_3 $t_{1/2} = 2$ hrs. producing 2-chloroacrolein
OH $t_{1/2} = 21$ hrs.
Photochemical degradation: reacts with reducing materials

Safety Hazard: Disaster hazard–dangerous chlorides

Chloroprene

PRODUCTION DATA

Annual U.S. Production: 396×10^6 lbs.

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 6.02

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{Lo}	1600 mg/kg	rat	oral
	500 mg/kg	rat	subcutaneous
	1000 mg/kg	mouse	subcutaneous
	300 mg/kg	cat	subcutaneous
	96 mg/kg	rabbit	intravenous
LC_{Lo}	600 mg/m^3 (8 hrs)	mouse	inhalation
	2500 mg/m^3 (8 hrs)	cat	inhalation

Non-lethal Acute Effects: 80 ppm

Central nervous system depression			
TC_{Lo} 80 ppm		human	inhalation

Degeneration of liver and kidneys
Dermatitis
Conjunctivitis–corneal necrosis
Anemia
Embryotoxic

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

TD_{Lo}	39 mg/m^3 (4 hrs per day for 48 days)	rat	inhalation

Teratogenicity:

TLV:

Other Chronic Effects:

Chloropropham

CHEMICAL NAME

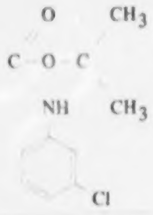
CAS Number: 101-21-3

Chemical Name: m-Chlorocarbanilic acid, isopropyl ester

Synonyms: Isopropyl-N-(3-chlorophenyl) carbanate
Isopropyl-m-chlorocarbanilate
Chloropropham

Molecular Formula: $C_{10}H_{12}ClNO_2$

Structure:



Chemical Properties

Molecular Weight: 213.7

Vapor Pressure:

Boiling Point: 247°C (decomposes)

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 36°C

Solubility:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Disaster hazard–dangerous toxic fumes of phosgene

Chloropropham

PRODUCTION DATA

Annual U.S. Production: 2×10^6 lbs.

Consumption:

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 2.0

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1200 mg/kg	rat	oral
	5000 mg/kg	rabbit	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Neoplasm	TD_{Lo}	60 mg/kg	mouse	oral

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

m-Chlorotoluene

CHEMICAL NAME

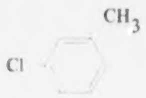
CAS Number: 108-41-8

Chemical Name: m-Chlorotoluene
3-Chloro-l-methylbenzene

Synonyms:

Molecular Formula: C_7H_7Cl

Structure:



Chemical Properties

Molecular Weight: 126.6

Vapor Pressure: 4.17 mm at 25°C

Boiling Point: 162.3°C

Density: 1.0797 at 13.90°C/4°C

Octanol/Water Partition Coefficient: 3.28

Physical State: Liquid

Vapor Density:

Melting Point: –48.0°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–slight

m-Chlorotoluene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

o-Chlorotoluene

CHEMICAL NAME

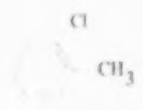
CAS Number: 95-49-8

Chemical Name: o-Chlorotoluene

Synonyms: 2-Chloro-1-methylbenzene
a-Chlorotoluene

Molecular Formula: C_7H_7Cl

Structure:



Chemical Properties

Molecular Weight: 126.6

Vapor Pressure: 4.11 mm at 25°C

Boiling Point: 159.3°C

Density:: 1.1018 at 0°C/4°C

Octanol/Water Partition Coefficient: 3.42

Physical State: Liquid

Vapor Density:

Melting Point: -35.1°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–slight

o-Chlorotoluene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1231 mg/kg	rat	oral
	1000 mg/kg	rat	subcutaneous
	1624 mg/kg	mouse	oral
Non-lethal Acute Effects:			
TC_{Lo}	16 ppm	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 1 ppm

Carcinogenicity: Neoplastic effects–TD_{Lo} 2100 mg/kg (51 weeks) rat subcutaneous

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

p-Chlorotoluene

CHEMICAL NAME

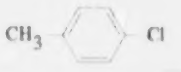
CAS Number: 106-43-4

Chemical Name: p-Chlorotoluene

Synonyms: 4-Chloro-l-methyltoluene
p-Tolylchloride

Molecular Formula: C_7H_7Cl

Structure:



Chemical Properties

Molecular Weight: 126.6

Vapor Pressure: 406 mm at 25°C

Boiling Point: 162.3°C at 760 mm

Density: 1.0697 at 20°C/4°C

Octanol/Water Partition Coefficient: 3.33

Physical State: Liquid

Vapor Density:

Melting Point: 7.5°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–slight

p-Chlorotoluene

PRODUCTION DATA

Annual U.S. Production: 95 x 10^6 lbs. (1976 capacity)

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Citric acid

CHEMICAL NAME

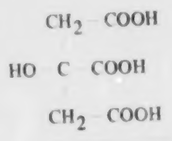
CAS Number: 77-92-9

Chemical Name: Citric acid

Synonyms: β-Hydroxytricarballylic acid
2-Hydroxy-1,2,3-propane tricarboxylic acid

Molecular Formula: $C_6H_8O_7$

Structure:



$$\begin{array}{l} \quad CH_2-COOH \\ HO\ \ C\ \ COOH \\ \quad CH_2-COOH \end{array}$$

Chemical Properties

Molecular Weight: 210.2

Vapor Pressure:

Boiling Point: Decomposes

Density: 1.542

Octanol/Water Partition Coefficient: 1.80

Physical State: Solid

Vapor Density:

Melting Point: 153°C

Solubility: 1,618 gm/l (H_2O)

Environmental Persistence

BOD: 53% of theoretical
Total theoretical oxygen demand gm/gm = 0.75

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 163.0 x 10^6 lbs.

Consumption: 152.4 x 10^6 lbs.

Fraction of Dispersion: 0.75

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 119.2

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	884 mg/kg	rat	intraperitoneal
	961 mg/kg	mouse	intraperitoneal
	42 mg/kg	mouse	intravenous
	330 mg/kg	rabbit	intravenous

Non-lethal Acute Effects:

Irritant with allergenic effects

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Crag herbicide 1

CHEMICAL NAME

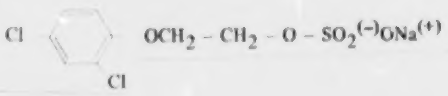
CAS Number: 136-78-7

Chemical Name: 2-(2,4-Dichlorophenoxy)ethanol, hydrogensulfate sodium salt

Synonyms:
Crag herbicide
Sesone
Sodium 2-(2,4-dichlorophenoxy)ethyl sulfate
Sodium 2,4-dichlorophenyl cellosolve sulfate

Molecular Formula: $C_8H_7Cl_2O_5S \cdot Na$

Structure:



Chemical Properties

Molecular Weight: 310.12

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 245°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Crag herbicide 1

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	730 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 15 mg/m^3

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

m-Cresol

CHEMICAL NAME

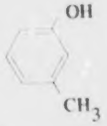
CAS Number: 108-39-4

Chemical Name: m-Cresol

Synonyms: m-Methylphenol
m-Hydroxytoluene

Molecular Formula: $CH_3C_6H_2OH$

Structure:



Chemical Properties

Molecular Weight: 108.1	**Physical State:** Liquid
Vapor Pressure: 1 mm at 52.0°C	**Vapor Density:** 3.72
Boiling Point: 202.8°C	**Melting Point:** 12°C
Density: 1.034 at 20°C/4°C	**Solubility:** Slightly soluble (H_2O)
Octanol/Water Partition Coefficient: 2.37	

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate
Explosion–moderate
Disaster hazard–dangerous toxic fumes

m-Cresol

PRODUCTION DATA

Annual U.S. Production: 31.4 x 10^6 lbs. (1973) (m and p cresol)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	242 mg/kg	rat	oral
	2050 mg/kg	rabbit	skin
LD_{Lo}	180 mg/kg	cat	subcutaneous
	1400 mg/kg	rabbit	oral
	280 mg/kg	rabbit	intravenous

Non-lethal Acute Effects:

CNS disorders
Kidney and liver damage
Irritation of skin and eyes

Chronic Toxicity

U.S. Occupational Standard: (air) TWA: 5 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 5 ppm

Other Chronic Effects:

o-Cresol

CHEMICAL NAME

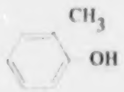
CAS Number: 95-48-7

Chemical Name: o-Cresol

Synonyms: o-Cresylic Acid
o-Hydroxytoluene

Molecular Formula: C_7H_8O

Structure:



Chemical Properties

Molecular Weight: 108.1

Vapor Pressure: 1 mm at 38.2°C

Boiling Point: 190.8°C

Density: 1.047 at 20°C/4°C

Octanol/Water Partition Coefficient: 3.40

Physical State: Solid

Vapor Density: 3.72

Melting Point: 30.9°C

Solubility: Soluble (H_2O) (31 gm/l)

Environmental Persistence

BOD: 95% of theoretical at 6 days
Toxic to sewage organisms

Atmospheric Reactivity: Reacts with oxidizing materials
Less than a day in air } Yields quinones and
Less than 10 days in water } benzenes

Safety Hazard: Fire–moderate
Explosion–slight
Disaster hazard–dangerous–toxic fumes

PRODUCTION DATA

Annual U.S. Production: 49.7 x 10^6 lbs.

Consumption: 49.7

Fraction of Dispersion: 0.3

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 15.6

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	121 mg/kg	rat	oral
	1100 mg/kg	rat	skin
	344 mg/kg	mouse	oral
	1380 mg/kg	rabbit	skin
LD_{Lo}	410 mg/kg	mouse	subcutaneous
	55 mg/kg	cat	subcutaneous
	940 mg/kg	rabbit	oral
	450 mg/kg	rabbit	subcutaneous
	180 mg/kg	rabbit	intravenous
	360 mg/kg	guinea pig	intraperitoneal
	200 mg/kg	frog	subcutaneous

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 5 ppm

Carcinogenicity: 20% benzene solution–papilloma in mouse

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects: Abnormal mitotic effects

p-Cresol

CHEMICAL NAME

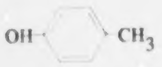
CAS Number: 106-44-5

Chemical Name: p-Cresol

Synonyms: 4-Cresol
4-Methylphenol
p-Hydroxytoluene

Molecular Formula: C_7H_8O

Structure:



Chemical Properties

Molecular Weight: 108.1

Vapor Pressure: 1 mm at 53.0°C

Boiling Point: 201.8°C

Density: 1.0341 at 20°C/4°C

Octanol/Water Partition Coefficient: 2.35

Physical State: Solid

Vapor Density: 3.72

Melting Point: 35.26°C

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate
Explosion–moderate
Disaster hazard–dangerous–toxic fumes

p-Cresol

PRODUCTION DATA

Annual U.S. Production: 31.4 x 10^6 lbs. (1973) (p and m cresol) **Consumption:**

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	207 mg/kg	rat	oral
	750 mg/kg	rat	skin
	344 mg/kg	mouse	oral
	301 mg/kg	rabbit	skin
LD_{Lo}	150 mg/kg	mouse	subcutaneous
	80 mg/kg	cat	subcutaneous
	620 mg/kg	rabbit	oral
	300 mg/kg	rabbit	subcutaneous
	180 mg/kg	rabbit	intravenous
	100 mg/kg	guinea pig	intraperitoneal
	150 mg/kg	frog	subcutaneous

Non-lethal Acute Effects:

Corrosive to skin and mucous membranes
Damage to kidney, liver, nervous system
Dermatitis

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 5 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity: TD_{Lo} 5500 mg/kg pregnant rat oral **TLV:** 5 ppm

Other Chronic Effects:

Crotonaldehyde

CHEMICAL NAME

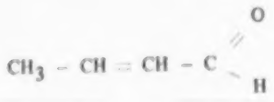
CAS Number: 123-73-9

Chemical Name: (E)-Crotonaldehyde

Synonyms: 2-Butenal
Crotonic aldehyde
β-Methyl acrolein

Molecular Formula: C_4H_6O

Structure:



$$CH_3 - CH = CH - C\begin{matrix} \diagup\!\!\diagup O \\ \diagdown H \end{matrix}$$

Chemical Properties

Molecular Weight: 70.09

Vapor Pressure: 10 mm at 25°C

Boiling Point: 104°C

Density: 0.853 at 20°C/20°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 2.41

Melting Point: -69°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD: 27% of theoretical at 10 days

Atmospheric Reactivity:. Reacts with oxidizing materials

Safety Hazard:

Crotonaldehyde

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	300 mg/kg	rat	oral
	140 mg/kg	rat	subcutaneous
	6 mg/kg	mouse	oral
	160 mg/kg	mouse	subcutaneous
	30	guinea pig	skin
LC_{50}	4000 mg/m^3 (30 minutes)	rat	inhalation
	1510 mg/m^3 (2 hours)	mouse	inhalation
Non-lethal Acute Effects:			
Irritant– TC_{Lo}	4 ppm	human	inhalation

Dangerous to eyes

Causes corneal burns, irritant to skin

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 2 ppm

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV: 2 ppm

Other Chronic Effects:

Crotonic acid

CHEMICAL NAME

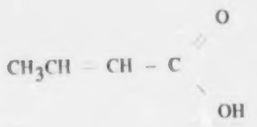
CAS Number: 324-65-0

Chemical Name: Crotonic acid

Synonyms: β-Methyl acrylic acid
Trans-2-butenoic acid
Methyl-propenoic acid

Molecular Formula: $C_4H_6O_2$

Structure:



$CH_3CH=CH-C\begin{matrix}\nearrow O\\ \searrow OH\end{matrix}$

Chemical Properties

Molecular Weight: 86.09

Vapor Pressure: 0.19 mm at 20°C

Boiling Point: 185°C

Density: 1.018 at 15°C/4°C

Octanol/Water Partition Coefficient: 0.76

Physical State: Solid

Vapor Density: 2.97

Melting Point: 72°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–slight

PRODUCTION DATA

Annual U.S. Production:	**Consumption:**
Fraction of Dispersion:	**Fraction of Production Lost:**
Release Rate (million lbs/yr):	

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1000 mg/kg	rat	oral
	600 mg/kg	guinea pig	skin

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity: **TLV:**

Other Chronic Effects:

Cumene

CHEMICAL NAME

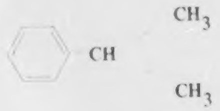
CAS Number: 98-82-8

Chemical Name: Cumene

Synonyms: Isopropyl benzene
2-Phenyl propane
Cumol

Molecular Formula: C_9H_{11}

Structure:



Chemical Properties

Molecular Weight: 120.21

Vapor Pressure: 6.56 at 25°C

Boiling Point: 152°C

Density: 0.864 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 4.1

Melting Point: -96°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD: 70% of theoretical for 20 days at 20°C
Total theoretical oxygen demand gm/gm = 3.5

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

Cumene

PRODUCTION DATA

Annual U.S. Production: 2292.9×10^6 lbs.

Consumption: 2737.2×10^6 lbs.

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 50.3

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1400 mg/kg	rat	oral
LC_{50}	8000 ppm	rat	inhalation
LC_{Lo}	2000 ppm	mouse	inhalation

Non-lethal Acute Effects:

Potent narcotic effects
Depressant to CNS
Dermatitis

Chronic Toxicity

U.S. Occupational Standard: (air): TWA 50 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Cumene hydroperoxide

CHEMICAL NAME

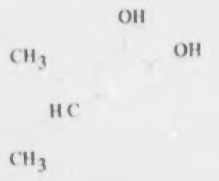
CAS Number: 80-15-9

Chemical Name: α,α-Dimethyl benzyl hydroperoxide

Synonyms: Caruacrol
o-Cresyl-5-isopropyl
2-Hydro-p-cumene

Molecular Formula: $C_9H_{12}O_2$

Structure:



Chemical Properties

Molecular Weight: 152.21

Vapor Pressure: 1 mm at 70°C

Boiling Point: 153°C

Density: 1.05

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point:

Solubility: Slightly soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Explosion–dangerous

Cumene hydroperoxide

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	382 mg/kg	rat	oral
	95 mg/kg	rat	intraperitoneal
	400 mg/kg	rat	subcutaneous
LD_{Lo}	5000 mg/kg	mouse	oral
	90 mg/kg	mouse	intraperitoneal
LC_{50}	220 ppm (4 hours)	rat	inhalation
	200 ppm (4 hours)	mouse	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Neoplastic effects:

TD_{Lo}	304 mg/kg	mouse	inhalation
	10 gm/kg (76 weeks)	mouse	subcutaneous

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Skin sensitizer

Cyanoacetic acid

CHEMICAL NAME

CAS Number: 372-09-8

Chemical Name: Cyanoacetic acid

Synonyms: Malonic acid, mononitrile

Molecular Formula: $C_3H_3NO_2$

Structure: $N \equiv C - CH_2 - COOH$

Chemical Properties

Molecular Weight:	85.06	Physical State:	Solid
Vapor Pressure:		Vapor Density:	
Boiling Point:	108°C at 15 mm	Melting Point:	66.1 to 66.4°C
Density:		Solubility:	Soluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Cyanoacetic acid

PRODUCTION DATA

Annual U.S. Production: 200 x 10^6 lbs. (1967)

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	200 mg/kg	mouse	intraperitoneal

Very toxic

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Cyanogen chloride

CHEMICAL NAME

CAS Number: 506-77-4

Chemical Name: Cyanogen chloride

Synonyms: Chlorine cyanide
CK

Molecular Formula: CClN

Structure: $Cl-C\equiv N$

Chemical Properties

Molecular Weight:	61.48	**Physical State:**	Liquid
Vapor Pressure:	1010 mm at 20°C	**Vapor Density:**	2.1
Boiling Point:	13.1°C	**Melting Point:**	-6.5°C
Density:	1.218 at 4°C/4°C	**Solubility:**	Soluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Cyanogen chloride

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	39 mg/kg	mouse	subcutaneous
	5 mg/kg	dog	subcutaneous
	20 mg/kg	rabbit	subcutaneous
LD_{50}	118 ppm (30 minutes)	rat	inhalation
	177 ppm (30 minutes)	mouse	inhalation
	207 ppm (30 minutes)	rabbit	inhalation
LD_{Lo}	207 ppm (30 minutes)	guinea pig	inhalation

Non-lethal Acute Effects:

Irritant to eyes and mucous membranes

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Cyanuric acid

CHEMICAL NAME

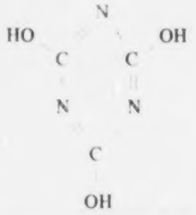
CAS Number: 108-80-5

Chemical Name: s-Triazine -2, 4, 6-triol

Synonyms:
sym-Triazinetriol
Tricyanic acid
Cyanuric acid, dihydrate
Tricarbimide

Molecular Formula: $C_3H_3N_3O_3$

Structure:



Chemical Properties (dihydrate)

Molecular Weight: 165.11

Vapor Pressure:

Boiling Point: decomposes

Density: 1.768 at 0°C

Octanol/Water Partition Coefficient:

Physical State: solid

Vapor Density:

Melting Point: 320 to 350°C (decomposes)

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Disaster hazard – cyanides

PRODUCTION DATA

Annual U.S. Production:	**Consumption:**
Fraction of Dispersion:	**Fraction of Production Lost:**
Release Rate (million lbs/yr):	

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
Highly toxic			

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity: TLV:

Other Chronic Effects:

Cyanuric chloride

CHEMICAL NAME

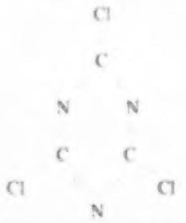
CAS Number: 108-77-0

Chemical Name: 2,4,6 Trichloro-s-triazine

Synonyms: Cyanuric chloride

Molecular Formula: $C_3Cl_3N_3$

Structure:



Chemical Properties

Molecular Weight:	184.42	Physical State:	Solid
Vapor Pressure:	2 mm at 70°C	Vapor Density:	6.36
Boiling Point:	190°C	Melting Point:	154°C
Density:	1.32 at 20°C/4°C	Solubility:	Insoluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Disaster hazard–dangerous–chlorides and nitriles

Cyanuric chloride

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	485 mg/kg	rat	oral

Non-lethal Acute Effects:

Irritation of mucous membranes
Disturbed heart rhythm

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Neoplastic effects

TD_{Lo}	22 gm/kg (82 weeks)	rat	oral
	750 mg/kg (15 weeks)	rat	subcutaneous

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Cyclohexane

CHEMICAL NAME

CAS Number: 110-82-7

Chemical Name: Cyclohexane

Synonyms: Hexahydrobenzene
Hexanapthene
Hexamethylene

Molecular Formula: C_6H_{12}

Structure:

Chemical Properties

Molecular Weight: 84.16

Vapor Pressure: 98.14 at 25°C

Boiling Point: 80.7°C

Density: 0.77855 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 2.90

Melting Point: 6.3°C

Solubility: Insoluble (H_2O) (<1 gm/l)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–dangerous
Explosion–moderate

Cyclohexane

PRODUCTION DATA

Annual U.S. Production: 416 x 10^6 lbs. (1976 capacity)

Consumption:

Fraction of Dispersion: 0.10

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 94.2 (1972)

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1297 mg/kg	mouse	oral
	5500 mg/kg	rabbit	oral
LD_{Lo}	77 mg/kg	rabbit	intravenous

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 300 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 300 ppm

Other Chronic Effects: Skin irritation
May be an asphyxiant

Cyclohexanol

CHEMICAL NAME

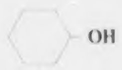
CAS Number: 108-93-0

Chemical Name: Cyclohexanol

Synonyms: Hexahydrophenol
Hexalin

Molecular Formula: $C_6H_{12}O$

Structure:



Chemical Properties

Molecular Weight: 100.17

Vapor Pressure: 1.7 mm at 25°C

Boiling Point: 161.5°C

Density: 0.9449 at 25°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 3.45

Melting Point: 23°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire - moderate

Cyclohexanol

PRODUCTION DATA

Annual U.S. Production: 760 x 10^6 lbs.

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.007

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2060 mg/kg	rat	oral
LD_{Lo}	1300 mg/kg	dog	oral
	800 mg/kg	cat	subcutaneous
	2200 mg/kg	rabbit	oral
	1420 mg/kg	rabbit	intraperitoneal

Non-lethal Acute Effects:

Mucous membrane effect: TC_{Lo} 100 ppm
Conjunctivitis
Corneal necrosis
Irritation of skin and respiratory tract

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 50 ppm

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV: 50 ppm

Other Chronic Effects: Damage to kidneys, liver, blood vessels

Cyclohexanone

CHEMICAL NAME

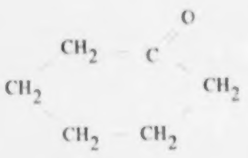
CAS Number: 108-94-1

Chemical Name: Cyclohexanone

Synonyms: Ketohexamethylene
Pimelic ketone
Hexanon
Cyclohexylketone

Molecular Formula: $C_6H_{10}O$

Structure:



Chemical Properties

Molecular Weight: 98.14	**Physical State:** Liquid
Vapor Pressure: 4.77 mm at 25°C	**Vapor Density:** 3.4
Boiling Point: 155.6°C	**Melting Point:** -47°C
Density: 0.9478 at 20°C/4°C	**Solubility:** 50 gm/l (H_2O)
Octanol/Water Partition Coefficient: 0.01	

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate
Explosion–slight

Cyclohexanone

PRODUCTION DATA

Annual U.S. Production: 784.4×10^6 lbs.

Consumption: 784.4

Fraction of Dispersion: 0.05

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 51.0

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1620 mg/kg	rat	oral
	1350 mg/kg	mouse	intraperitoneal
LD_{Lo}	1000 mg/kg	rabbit	skin
	1300 mg/kg	mouse	oral
	630 mg/kg	dog	intravenous
	1600 mg/kg	rabbit	oral
LC_{Lo}	2000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Irritant: eyes and throat

TC_{Lo}	50 ppm	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 50 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 50 ppm

Other Chronic Effects:

Cyclohexene

CHEMICAL NAME

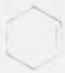
CAS Number: 110-83-8

Chemical Name: Cyclohexene

Synonyms: 1,2,3,4-Tetrahydrobenzene

Molecular Formula: C_6H_{10}

Structure:



Chemical Properties

Molecular Weight: 82.14

Vapor Pressure: 160 mm at 38°C

Boiling Point: 83°C at 760°C

Density: 0.8102 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 2.8

Melting Point: -103.7

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–dangerous

Cyclohexene

PRODUCTION DATA

Annual U.S. Production: 2298.4 x 10^6 lbs.

Consumption: 1779.4

Fraction of Dispersion: 0.04

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 94.2

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 300 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Cyclohexylamine

CHEMICAL NAME

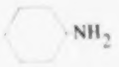
CAS Number: 108-91-8

Chemical Name: Cyclohexylamine

Synonyms: Hexahydroaniline
Aminocyclohexane

Molecular Formula: $C_6H_{13}N$

Structure:



Chemical Properties

Molecular Weight: 99.2	**Physical State:** Liquid
Vapor Pressure:	**Vapor Density:** 3.42
Boiling Point: 134.5°C	**Melting Point:** -18°C
Density: 0.865 at 25°C/25°C	**Solubility:** Soluble (H_2O)
Octanol/Water Partition Coefficient:	

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate
Disaster hazard–dangerous–toxic fumes

Cyclohexylamine

PRODUCTION DATA

Annual U.S. Production: 12 x 10^6 lbs. (1967)

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	710 mg/kg	rat	oral
	200 mg/kg	rat	intraperitoneal
	300 mg/kg	mouse	intraperitoneal
	320 mg/kg	rabbit	skin
LD_{Lo}	500 mg/kg	rabbit	parenteral
LC_{Lo}	8000 ppm (4 hours)	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 10 ppm

Other Chronic Effects: Dermatitis
Convulsions
CNS depression

Cyclopentadiene

CHEMICAL NAME

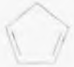
CAS Number: 542-92-7

Chemical Name: 1,3-Cyclopentadiene

Synonyms:

Molecular Formula: C_5H_6

Structure:



Chemical Properties

Molecular Weight: 66.11	**Physical State:**
Vapor Pressure: 10 mm at 25°C	**Vapor Density:**
Boiling Point: 40.0°C at 760 mm	**Melting Point:** -97.2°C
Density: 0.80475 at 19°C/4°C	**Solubility:** Insoluble (H_2O)
Octanol/Water Partition Coefficient:	

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate
Explosion–moderate

Cyclopentadiene

PRODUCTION DATA

Annual U.S. Production: 100 x 10^6 lbs. (Total capacity)

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
TD_{Lo}	250 ppm	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 75 ppm

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects: Abdominal pain
Jaundice
Anemia

Cyprex

CHEMICAL NAME

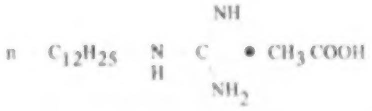
CAS Number: 2439-10-3

Chemical Name: Dodecylguanidine, monoacetate

Synonyms: Cyprex
Dodine

Molecular Formula: $C_{13}H_{29}N_3.C_2H_4O_2$

Structure:



$\text{n } C_{12}H_{25}\ \underset{H}{N}\ \overset{NH}{\underset{NH_2}{C}} \bullet CH_3COOH$

Chemical Properties

Molecular Weight: 287.36

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 136°C

Solubility: Soluble (hot H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 2.0×10^6 lbs.

Consumption: 2.0×10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 2.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	566 mg/kg	rat	oral
	1000 mg/kg	rat	unknown

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Strong solutions cause severe irritation of skin and eyes

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